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Interim User's Guide to the RADM Scavenging Module Version 1.0

Battelle Pacific Northwest Labs., Richland, WA

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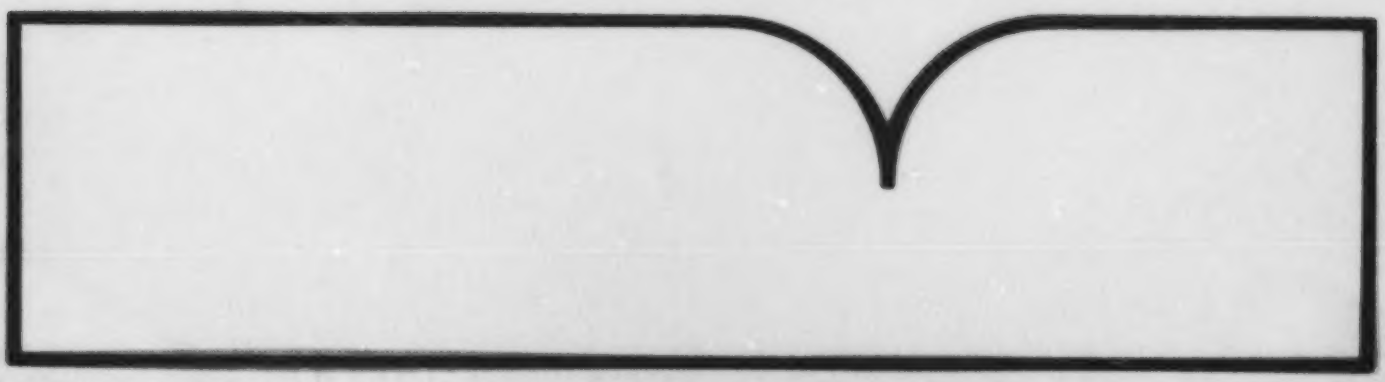

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INTERIM USER'S GUIDE TO THE RADM SCAVENGING MODULE
Version 1.0

by

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Using surface precipitation rates and vertical profiles of temperature and moisture for a regional scale grid square, the scavenging module calculates steady-state cloud, precipitation and vertical velocity fields for subgrid areas representing stratiform, convective and fair weather cumulus clouds. It then calculates the effects of aqueous phase chemistry, precipitation scavenging and transport on the pollutant fields presented by the host code for a specified time period (one hour).

The version of the RSM described in this report includes the stratiform and convective storm component; it does not include the fair weather cumulus (although provisions for including this component are outlined). A description of several proposed benchmark tests is provided; the results of these tests will be published in future reports.

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SECTION 1

INTRODUCTION

This report presents an interim user's manual for Version 1.0 of the RADM Scavenging Module (RSM). The RSM is embodied in a set of FORTRAN subroutines that, when interrogated by a regional-pollution "host" code, compute

- pollutant removal by precipitation scavenging,
- pollutant transformation by aqueous-phase chemical processes,
- pollutant redistribution in storm systems by vertical-transport processes and
- precipitation-borne pollutant delivery to the surface.

The RSM has been prepared specifically to operate with the Regional Acid Deposition Model (RADM) host code. The RADM is currently being developed at the National Center for Atmospheric Research, funded by the Environmental Protection Agency and coordinated by the National Acid Precipitation Assessment Program Task Force.

Technical features of the RSM can be considered to fall into the following individual categories:

- interties and communication linkages between the RSM and the RADM,
- treatment of meteorological variability of scavenging systems within the 80 by 80 km RADM horizontal grid, and
- treatment of physical and chemical phenomena within the structure of the RSM.

This user's manual has been formatted to discuss each of these categories in several progressive stages. Section 1 is intended to provide an initial overview to enable the reader to grasp global features of the RSM without becoming immersed in fine details of actual module operations. Subsequent

sections will describe the module in increasing detail with the intent of providing the user with the hands-on operating skills necessary for actual execution of the code. This initial discussion is presented sequentially in the following subsections.

1.1 RSM/RADM INTERTIES

In the absence of a scavenging module the RADM is simply an advanced clear-air regional pollution code, which operates in an Eulerian frame of reference over an extensive 80 by 80 km mesh grid. For purposes of discussion this will be referred to as the "dry-RADM." The dry-RADM simulates three-dimensional transport, clear-air chemistry, emissions, and dry deposition. Meteorological data is provided by the Mesoscale Meteorological Model (MM4) of Anthes (1985).

In contrast, the RSM deals with all processes related to clouds and precipitation (see Figure 1). The interaction between the two is roughly as follows:

1. The dry-RADM computes transport and clear-air chemistry for a one-hour period.

2. The RSM is then activated at each "grid-column." A grid-column is the vertical column over a particular RADM surface grid point. In activating the RSM, the RADM/MM4 system provides

   - vertical profiles of temperature, moisture and updraft velocities;
   - convective precipitation amount for the past hour; and
   - vertical profiles of clear-air pollutant species (gases and aerosols).

3. Fields of cloud and precipitation consistent with these profiles are established by the RSM. The effects of precipitation scavenging, aqueous chemical transformations and vertical transport by sub-grid (convective) motions for one hour are then calculated.

4. At the end of an hour, pollutants in the RSM exist as gases and aerosols. Pollutants also exist in cloud, rain and snow media. The RSM combines the vertical profiles of these different forms of each pollutant (e.g., sulfate) to produce an "equivalent clear-air profile." These profiles are returned to the RADM, along with surface wet deposition amounts for pollutants that have been scavenged.

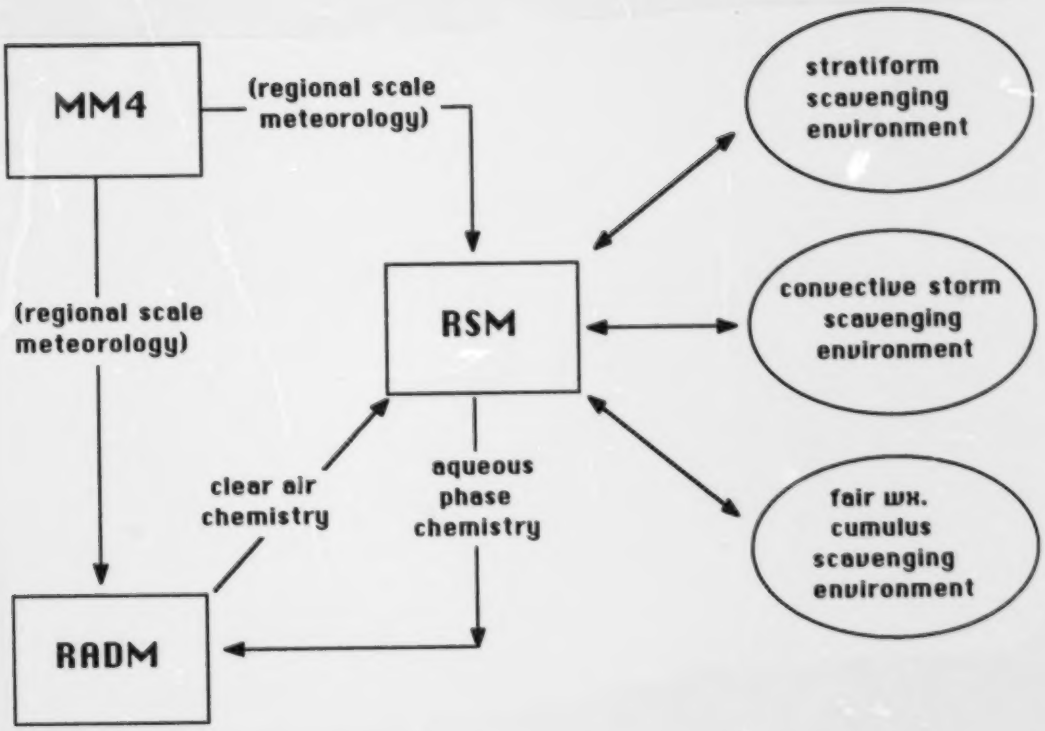


Figure 1. Illustration of calling hierarchy between RADM, and RADM scavenging module (RSM), MM4, the precipitating stratiform model, the precipitating convective storm model, and the fair weather cumulus model.

5. The effects of clouds and precipitation for one hour are represented by the change between the initial profiles passed to the RSM from the RADM and the equivalent clear-air profiles the RSM passes back to RADM. RADM combines this change with those computed in Step 1 and then proceeds to the next one-hour simulation.

Two points should be emphasized. First, the RSM operates on one RADM grid-column at a time. All horizontal interactions between grids are handled in dry-RADM; none occur in the RSM. Secondly, the RSM is initialized each hour; it does not "remember" the profiles of, for example, sulfate in cloud and rain from the end of the previous hour. This has required a special initialization procedure be developed for the RSM.

1.2 SUB-GRID VARIABILITY

The 80 by 80 km horizontal grid spacing of the RADM offers ample opportunity for multiple cloud and storm features to coexist within a single grid element. This is particularly true for convective-storm and cloud phenomena and has necessitated some specialized parameterization techniques within the RSM. The basic approach applied by the RSM to deal with this problem is outlined as follows:

- Within a given RADM horizontal grid, clouds, clear air, and precipitating systems are segregated into several classes (precipitating and nonprecipitating stratus, precipitating and nonprecipitating cumulus, clear air). Multiple elements within these classes are presumed to be represented by a single simulated entity.

- A "grid column" is defined as the vertical volume above the 80 by 80 horizontal grid square where model computations are currently in progress.

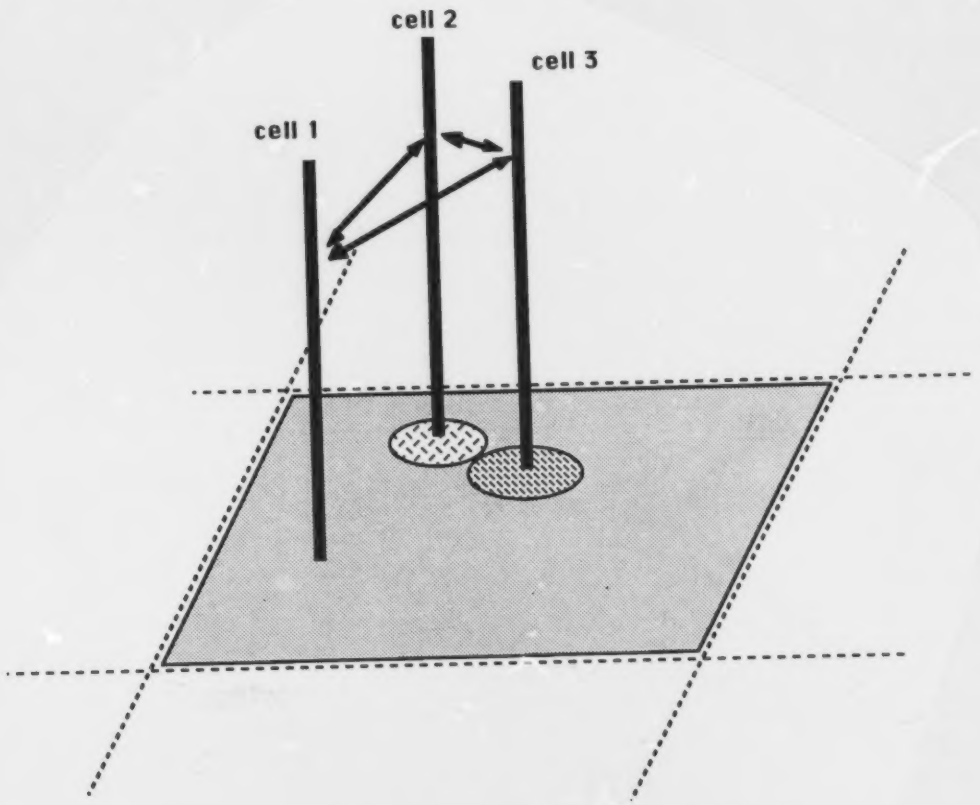
- Meteorological data from the RADM/MM4 system is used to determine the types, sizes, and intensities of the storm classes within this grid column.

- The grid column is filled with up to four "cells", which define the spatial boundaries of the chosen storm classes or "operator clouds."

- Macroscopic material balances are performed over the defined cells, starting with microscopic equations for pollutant conservation. These equations contain terms for inflow/outflow at the cell interfaces, thus linking the individual simulations.

- Numerical approximations are made to the solutions of the material-balance equations. The resulting chemical-species concentrations are reapportioned to the RADM as described above.

A schematic of a typical grid column and cells ("operator-cloud" boundaries) is shown in Figure 2. In this particular example, cell 1 covers the total grid column except for the cylindrical volumes occupied by cells 2 and 3. Inflows and outflows through the cell interfaces are represented by the horizontal arrows. The cell/column arrangement indicated by Figure 2 is of central importance to the RSM. This schematic should be borne in mind as the reader proceeds to the more detailed sections of this report.



Note:
Solid vertical lines indicate vertical domain of individual operator clouds.
Dashed lines indicate boundary of RADM grid.
Shaded areas indicate areal extent of operator clouds.
Cell 1 encompasses total area not covered by cells 2 and 3.

Figure 2. Schematic of operator clouds within a RADM grid.

1.3 INTERNAL TREATMENT OF PHYSICAL AND CHEMICAL PHENOMENA

Two features of internal RSM operations should be noted at this overview stage of the presentation. The first of these is that the RSM is basically a stand-alone model which, with some modification, could be made to operate independently as a pollution host code. It performs numerical integrations of species-conservation equations which are similar to those of the RADM, the main differences being that they allow for multiple aqueous as well as gaseous media and that their dimensionality is restricted. The RSM has been derived directly from the PLUVIUS-series reactive-storm codes and employs the numerical integration techniques developed for PLUVIUS II.

The second important feature of the RSM is its application of PLUVIUS-based "interaction-diagram" concepts to simulate multiple chemical and microphysical phenomena. Described in detail in later sections of this report, the RSM's interaction-diagram based structure allows for substantial mechanistic reality and versatility. This is a particularly important feature because it permits direct input from other Task Force activities, which are currently in the process of improving mechanistic understanding of fundamental scavenging processes.

1.4 PRESENT STATUS OF THE RSM

Version 1.0 of the RSM represents a working code, which can be applied directly as a module for scavenging calculations. It should be considered as an evolving code, however, which will be modified substantially with the advancement of time, external developments, and operating experience. Specific points in this regard are noted as follows

- The RADM is an immature and changing code and thus the intertie protocols between the RSM and the RADM have not been firmly established. For benchmarking and other testing purposes this difficulty has been partly offset by writing a local "RADM emulator", which interrogates the RSM as if it were the actual host code. The RADM emulator is included with interim RSM Version 1.0 and substantial effort is planned for formal RADM interties in the immediate future. This will undoubtedly alter the structure of Version 1.0 somewhat.

- The RSM depends on some external activities which are incomplete at the present time. For example, the nonprecipitating cumulus cloud sub module is currently inactive, but anticipates external developments in this area. Version 1.0 can be expected to be updated as these results become available.

- The RSM is based heavily on the reactive storm models PLUVIUS MOD 5.0 and PLUVIUS II. MOD 5.0 is a mature code and has been documented in user's manual form. PLUVIUS II is still in an evolving stage, however, and while it has been tested fairly rigorously, its benchmark tests will not be reported in user-manual form for at least one year. This presents a minor tracability problem, which is common to many developmental projects using evolving technologies.

- As noted above, the interaction-diagram core of the RSM has been designed to accommodate advancements in mechanistic understanding as these advancements emerge from other Task Force elements. The Processing of Emissions by Clouds and Precipitation (PRECP)

program, for example, plans to create a progressive series of three interaction-diagram sets between 1986 and 1988, which are intended specifically for incorporation within the RSM. Future RSM versions can be expected to evolve accordingly.

In summary, Version 1.0 of the RSM is presented as a working module which is expected to evolve significantly during the next two years and this initial user's manual is viewed as a tool to facilitate this process.

The following sections provide a detailed description of the features embodied by this initial version of the code.

SECTION 2

KEY TECHNICAL FEATURES OF THE RSM

2.1 RSM GOVERNING EQUATIONS

The task of the RSM is to simulate the effects of clouds and precipitation on pollutant species for a specified time period (currently one hour) within a "grid-column" of horizontal dimensions of 80 by 80 km and vertical dimension of up to 10 km. Up to four operator clouds may be defined within this area. An operator cloud is defined to be a single cloud element that characterizes a population of such elements. Figure 2 illustrates one such example, wherein there are three operator clouds. Depending on environmental conditions specified by the RADM/MM4 system, up to four such operator clouds (or cells) may be defined. Pollutant species concentrations are computed as a function of time, height and cell by solving a set of conservation equations for the species. In this section, we derive the governing conservation equations.

The starting point is the 3-dimensional conservation equation for a pollutant species:

$$\frac{\partial c_s}{\partial t} = - \nabla_H \cdot (V_H c_s) - \frac{\partial}{\partial z} \left[(w_a + w_{fs}) \, c_s \right] + \text{Turbxy}_s + \text{Turbz}_s + G_s \, , \qquad (1)$$

where c_s (x,y,z,t) = concentration (moles/cm^3) of species "s"

V_H (x,y,z) = horizontal air velocity (since the operator clouds are steady state for the one hour period, V_H and other transport variables are also steady state)

w_a (x,y,z) = vertical air speed

w_{fs} (x,y,z) = fall speed for species "s" (non-zero for rain and snowborne species)

Turbxy = horizontal turbulent transport of the species (assumed to be described by K-theory),

Turbz = vertical turbulent transport, approximated using K-theory.

$$\text{Turbz}_s = \frac{\partial}{\partial z}\left[c^* K_{zzs} \frac{\partial}{\partial z}\left(\frac{c_s}{c^*}\right)\right] ,$$

where K_{zzs} = vertical eddy transport coefficient for species "s." It includes both the effect of turbulent air motions and pseudo-diffusion resulting from precipitation particle size distributions (see Easter and Hales 1984).

Also, $c^*(z)$ = air concentration (mole/cm^3), which is assumed to be horizontally uniform within the grid column.

$G_s\ (x,y,z,t)$ = generation rate for species "s," including source and sink terms describing chemical transformations and physical scavenging.

A basic approximation of the RSM is that pollutant concentrations within the grid-column can be adequately characterized by their horizontal averages within each cell. Thus we define

$$c_{sj}\ (z,t) = \frac{1}{A_j} \iint_{\text{cell } j} dx\ dy\ c_s , \qquad (2)$$

where s is a chemical species index, j is the cell index (identifying each operator cloud) and A_j is the horizontal area of cell j. Conservation equations for c_s are obtained by horizontal averaging of terms in Equation 1.

For the temporal derivative, one has[1]

$$\frac{\partial c_{sj}}{\partial t} \equiv \frac{1}{A_j} \iint dx\ dy \frac{\partial c_s}{\partial t} , \qquad (3)$$

because the cell areas are fixed during each RSM activation.

---

[1]In this text, all double integrals are intended to signify the domain of cell j.

For the vertical advection term, one defines

$$w_{aj}(z) = \frac{1}{A_j} \iint dx\, dy\, w_a ,$$

$$w_{fs}(z) = \frac{1}{A_j} \iint dx\, dy\, w_{fs} .$$

Next one defines deviations from the cell averages by

$$w_a = w_{aj} + w_a' ,$$

$$w_{fs} = w_{fsj} + w_{fs}' ,$$

$$c_s = c_{sj} + c_s' .$$

Then

$$\frac{1}{A_j} \iint dx\, dy\, (w_a + w_{fs})\, c_s = (w_{aj} + w_{fsj})\, c_{sj} + \frac{1}{A_j} \iint dx\, dy\, (w_a' + w_{fs}')\, c_s' .$$

For this and other terms, the correlations between the primed quantities are ignored to obtain:

$$\frac{1}{A_j} \iint dx\, dy\, (w_a + w_{fs})\, c_s \tilde{=} (w_{aj} + w_{fsj})\, c_{sj} \qquad (4)$$

The horizontal turbulent transfer term, $Turbxy_s$ is ignored. This means that turbulent transport between cells is ignored. The simple models of operator clouds ignore this transfer, although they do account for dynamic entrainment and detrainment.

For the vertical turbulent transfer term one defines

$$K_{zzs_j}(z) = \frac{1}{A_j} \iint dx\, dy\, K_{zzs}$$

and approximates (neglecting primed terms)

$$\text{Turbz}_{sj} = \frac{1}{A_j} \iint dx\, dy \frac{\partial}{\partial z}\left[c^* K_{zzs} \frac{\partial}{\partial z}\left(\frac{c_s}{c^*}\right)\right] \simeq \frac{\partial}{\partial z}\left[c^* K_{zzs_j} \frac{\partial}{\partial z}\left(\frac{c_{sj}}{c^*}\right)\right]. \quad (5)$$

The generation term G_s generally has the form

$$G_s\,(x,y,z,t) = G_s\,[c_1\,(x,y,z,t),\ c_2\,(x,y,z,t),\ \ldots]$$

since reaction and scavenging rates depend on the concentration of various species. The approximation for this term is

$$G_{sj} = \frac{1}{A_j} \iint dx\, dy\, G_s\,(c_1\, c_2, \ldots) \simeq G_s\,(c_{1j}, c_{2j}, \ldots)\,. \quad (6)$$

For the horizontal advection term, we define

$$\text{HOR}_{sj} = -\frac{1}{A_j} \iint dx\, dy\, \nabla_H \cdot (V_H\, c_s).$$

This can be transformed using the two-dimensional form of the divergence theorem to give:

$$\text{HOR}_{sj} = -\frac{1}{A_j} \oint ds\, \hat{n}_j \cdot V_H\, c^* \left(\frac{c_s}{c^*}\right), \quad (7)$$

where this line-integral is evaluated around the boundary of cell j, and $\hat{n}_j$ is the unit vector outward-normal to the boundary. In this form, one sees that HOR_{sj} is determined by the transport of the species across the cell boundary.

To develop this further, note that the boundary of cell j consists of sections where cell j is adjacent either to another cell or to the grid-column boundary. A section of the boundary where cell j is adjacent to cell m can be divided into two subsections: an outflow subsection where air flows out of cell j into cell m, and an inflow subsection, where air flows into cell j from cell m. With this picture one can write

$$\oint ds\ \hat{n}_j \cdot V_H\ c^* = \sum_{m \neq j} (F_{jm} - F_{mj}) , \tag{8}$$

$$\oint ds\ \hat{n}_j \cdot V_H\ c_s = \frac{1}{c^*} \sum_{m \neq j} (F_{jm}\ c_{sj} - F_{mj}\ c_{sj}) , \tag{9}$$

where for cell j, the summations are for all m for m = 1, 2, ..., m not equal to j, and

F_{mj} = the portion of $\oint ds\ \hat{n}_j \cdot V_H\ c^*$ where cells j and m are adjacent and air is flowing out of cell j into cell m. The approximation is made that on this portion of the cell j boundary, c_s is represented by c_{sj}.

Also, $-F_{mj}$ = the portion of the integral where cells j and m are adjacent and air is flowing into cell j from cell m. On this portion of the boundary one approximates c_s by c_{sm}.

With this one can write

$$HOR_{sj} = -\frac{1}{c^*\ A_j} \sum_{m \neq j} (F_{jm}\ c_{sj} - F_{mj}\ c_{sm}) . \tag{10}$$

Thus, the net horizontal transport consists of a set of inflows from and outflows to adjacent cells.

One can now write the conservation equation for a cell by combining Equations 3, 4, 5, 6, and 10:

$$\frac{\partial c_{sj}}{\partial t} = -\frac{1}{c^*\ A_j} \sum_{m \neq j} (F_{jm}\ c_{sj} - F_{mj}\ c_{sm}) - \frac{\partial}{\partial z}\left[(w_{aj} + w_{fsj})\ c_{sj}\right] + \frac{\partial}{\partial z}\left[c^*\left(K_{zzsj}\frac{\partial}{\partial z}\ \frac{c_{sj}}{c^*}\right)\right] + G_{sj} . \tag{11}$$

This equation needs one additional term, Q_{sj}. This term represents transport between cells by processes other than horizontal advection. In the two-cell (updraft, downdraft) precipitating convective cloud model used in the RSM, there is additional transfer (besides HOR_{sj}) of rain and snow from the updraft operator cloud (j=2) to the downdraft operator cloud (j=3) (Scott 1986b)[1]. This transfer process will also transfer rain and snowborne pollutants and leads to the following terms

$$Q_{s2} = - \beta_{s23} \, c_{s2} \, ,$$

$$Q_{s3} = + \frac{A_2}{A_3} \beta_{s23} \, c_{s2} \, , \tag{12}$$

where β_{s23} is determined by the transfer rate out of the updraft cell and is nonzero only for rain and snowborne species. With this, one has

$$\frac{\partial c_{sj}}{\partial t} = (\text{right hand side of Eq. 11}) + Q_{s2} \, . \tag{13}$$

Because the PLUVIUS II reactive scavenging code uses mixing ratios,

$$r_{sj} = \frac{c_{sj}}{c^*} \, ,$$

the conservation equations will also be written in mixing ratio form:

$$\frac{\partial r_{sj}}{\partial t} = - \frac{1}{c^* A_j} \sum_{m \neq j} (F_{jm} \, r_{sj} - F_{mj} \, r_{sm}) - \frac{1}{c^*} \frac{\partial}{\partial z} \left[c^* (w_{aj} + w_{fsj}) \, r_{sj} \right]$$

$$+ \frac{1}{c^*} \frac{\partial}{\partial z} \left(c^* \, K_{zzsj} \frac{\partial}{\partial z} r_{sj} \right) + \frac{1}{c^*} G_{sj} + \frac{1}{c^*} Q_{sj} \, . \tag{14}$$

Equations 13 and 14 are the governing equations of the RADM Scavenging Module.

---

[1] Scott, B. C. 1986b. "User's Manual for the Convective Storm Component of the RSM." (In preparation.)

The parameters which describe transport within and between the cloud/storm cells (w_{aj}, w_{fj}, F_{jm}, and F_{mj}) are established by the cloud models used in the RSM. These parameters are constrained by the environmental conditions specified by the host code (RADM) and by the fact that the RADM itself computes 3-D transport of clear air pollutant species. Three of these constraints should be emphasized.

1. The RADM calculates all transport between grid columns; none is calculated by the RSM. This means that the horizontal transfer terms involving Cell 5 (the area outside a grid column) are ignored, not because they are zero, but because RADM has already taken them into account.

2. The RADM calculates vertical advection and mixing, using its regional scale vertical velocity and eddy transfer coefficients. Thus, the w_{aj} and K_{zzsj} used in RSM should have the RADM values (w_{host} and K_{zzhost}) subtracted from them. This is done in all cells except those convective cells in which

$$|w_{aj}| >> |w_{host}| .$$

3. For mass consistency with the RADM vertical velocity fields, the RSM should have a net mass flux equal to that of RADM/MM4. Letting V = volume of an operator cloud, and A_j be the cross sectional area, then

$$(c^* V)_{RADM} = (c^* V)_{RSM}$$

$$\left(\sum A_j\right) w_{a,RADM} = \sum \left(A_j w_{aj}\right)_{RSM} , \qquad (15)$$

where $w_{a,RADM}$ is the vertical air speed defined by the host, and w_{aj} is the vertical air speed within cell j.

2.2 LATERAL EXCHANGE PROCESSES

Lateral exchange (horizontal transport) occurs between cells whenever more than one cell exist in the grid-column. The possible combinations of operator clouds allowed in the RSM are listed in Table 1, along with cell definitions for each case. These cases are illustrated in Figure 3.

Table 1. CLOUD/STORM COMBINATIONS ALLOWED IN RSM (OTHER THAN NO CLOUDS) AND ASSOCIATED CELL DEFINITIONS

Case	Cell 1	Cell 2	Cell 3	Cell 4
1. Stratiform only	St updraft	--	--	--
2. Precipitating convective only	Clear-air	Cb updraft	Cb downdraft	--
3. Nonprecipitating convective only	Cu updraft	--	--	Cu subsidence
4. Stratiform and precipitating convective	St updraft	Cb updraft	Cb downdraft	--
5. Precipitating and nonprecipitating convective	Cu updraft	Cb updraft	Cb downdraft	Cu subsidence

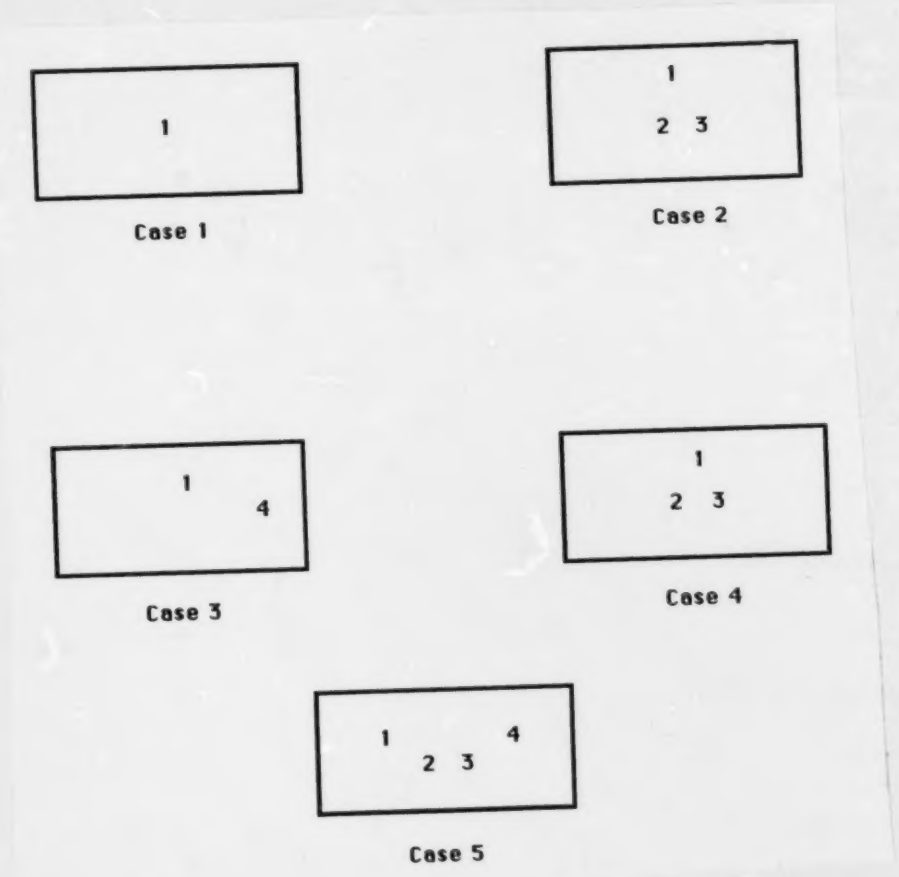


Figure 3. Cell definition for different RSM cases.

The lateral exchange rates (the F_{jm}) are determined by the precipitating and nonprecipitating convective cloud models and represent dynamic entrainment and detrainment processes. For the nonprecipitating convective cloud, exchange occurs between the updraft cell and the subsidence cell and is determined by the Vukovich fair weather cumulus model. For the precipitating convective cloud, exchange occurs between 1) the updraft and downdraft cells, 2) between the updraft cell and a surrounding "buffer" cell, and 3) between the downdraft cell and the buffer cell and all are determined by Scott's (1986b) model. For Cases 2 and 3 (Table 1), the buffer cell is Cell 1. For Case 5, the buffer cell is Cell 4. One notes that for Case 2, the precipitating convective cloud only, a special clear-air cell must be established, because the convective cloud updraft and downdraft cells occupy only about 10% of the grid-column.

The lateral exchange rates are largely determined by the continuity equation for air,

$$\frac{\partial c^*}{\partial t} = - \nabla_H \cdot (V_H \, c^*) - \frac{\partial}{\partial z} (w_a \, c^*) \, ,$$

which reduces to

$$\nabla_H \cdot (V_H \, c^*) = - \frac{\partial}{\partial z} (w_a \, c^*) \, ,$$

as one assumes c* is a function of z only. To this last relation, one applies the horizontal averaging over a cell to obtain (by Equation 8)

$$\frac{1}{A_j} \iint dx \, dy \, \nabla_H \cdot V_H \, c^* = \frac{1}{A_j} \sum_{m \neq j} (F_{jm} - F_{jm})$$

and

$$\frac{1}{A_j} \iint dx \, dy \, \frac{\partial}{\partial z} (w_a \, c^*) = \frac{\partial}{\partial z} (w_{aj} \, c^*) \, .$$

Thus

$$\frac{1}{A_j} \sum_{m \neq j} (- F_{jm} + F_{mj}) = + \frac{\partial}{\partial z} (w_{aj} \, c^*) \, . \qquad (16)$$

For the nonprecipitating (fair weather) convective cloud, one applies Equation 16 to Cell 1 (the updraft) and assumes that Cell 1 interacts only with Cell 4. This gives

$$\frac{1}{A_1} (- F_{14} + F_{41}) = \frac{\partial}{\partial z} (w_{a1} \, c^*) \, .$$

When the right hand side is positive (entrainment), one specifies $F_{14} = 0$; when the right hand side is negative (detrainment), one specifies $F_{41} = 0$, thus, transfer to and from the fair weather updraft cell is defined.

For the precipitating convective cloud, one applies Equation 16 to both the updraft and downdraft cells. This case is more complex, however, as transfer occurs between 3 cells. Thus, one must make additional assumptions, such as how much of the updraft cell entrainment comes from the buffer cell versus the downdraft cell. This is discussed further in Scott (1986b).

2.3 CALCULATION OF THE UPDRAFT IN THE STRATIFORM REGION

As discussed on page 12 (Equation 15), for the RSM to be consistent with the host code, the RSM vertical velocity, averaged over the RSM cells, should equal the host code vertical velocity. This can be written as

$$w_{a,host} = \sum_{1}^{4} a_j \, w_{aj} \, ,$$

where,

$$a_j = \frac{A_j}{\sum_{1}^{4} A_j} \, ,$$

is the fractional area for Cell j. For the cases in which the stratiform cloud is present, the vertical velocity in this cell should satisfy

$$w_{a,St} = \frac{1}{a_{St}} \, w_{a,host} - \sum_{j \neq St} a_j \, w_{aj} \, , \qquad (17)$$

where "St" refers to the stratiform cloud cell. This would uniquely determine the stratiform w_a, since either the stratiform cloud is present alone, or else it exists with the precipitating convective cells where w_a's are determined by the convective precipitation amount.

The updraft profile resulting from Equation 17 can be very "ill-mannered" and constraints imposed by the numerics of the stratiform model of Scott require a second transformation in defining the stratiform updraft of the RSM. This transformation of the values from Equation 17 is necessary to assure a smooth, positive valued profile for the stratiform model. Discontinuous or non-monotonically changing updraft profiles produce unrealistic results in this component of the RSM. This problem arises from the assumption that all cloud water at a given layer is generated from below.

To assure that this problem does not develop during use of the RSM, w_{St} is characterized within the RSM by a parabolic profile having the <u>same vertical average</u> value as w_{St} identified by Equation 17:

$$\langle w_{St} \rangle = \frac{1}{H} \int w_{a,St} \, (z) \, dz \, , \qquad (18)$$

where the stratiform cloud top height, H, is defined by the first layer above the freezing level at which $w_{nonconv} \leq 0.015$ cm/s. The temperature criteria for cloud top height is a restriction imposed by the nucleation mechanism assumed within the stratiform cloud model (namely, that precipitation embryos are assumed to be ice crystals which grow at the top of the cloud by vapor deposition). The updraft at a height z within the stratiform region is then given by

$$w'_{St} = \frac{6 \langle w_{St} \rangle}{H} z \ (1 - z/H) \tag{19}$$

The stratiform updraft field defined by this algorithm approximately conserves mass over the vertical extent of this column since the average flux over a column is

$$\langle flux \rangle = (1/H) \int w \ c^* \ dz \ . \tag{20}$$

This in turn can be approximated by

$$\langle flux \rangle \approx \langle w \rangle \ \langle c^* \rangle \ , \tag{21}$$

where $\langle w \rangle$ is given by by Equation 18.

The updraft defined in Equation 19 is used only in defining the cloud environment of the widespread stratiform operator cloud. It is not used to calculate either vertical transport or lateral inflow of pollutant species in the stratiform cloud. These processes are assumed to be simulated by the host code.

2.4 MASS BUDGET OF AN OPERATOR CLOUD

A quantitative statement describing the mass budget of the RSM can be derived beginning with the pollutant mass continuity equation (Equation 14). Multiplying this expression by c* (which is assumed to be steady state), integrating over height and time, and evaluating at the top and bottom of the operator cloud (or "cell") the terms that are exact differentials of height ($\partial/\partial z$), results in an expression that evaluates the total change in mass for any region of the model independently from the detailed microphysics, scavenging and chemistry. Letting M (moles/cm^2) denote the total mass per unit area in cell j at time t, one has:

$$M_s(t=\delta t) - M_s(t=0) =$$

$$\int_0^{\delta t} dt \left\{ -\int_0^H \frac{1}{A_j} \sum_{j \neq m} (F_{jm} r_{sj} - F_{mj} r_{sm})\, dz \right.$$

$$- c^* (w_{aj} + w_{fsj}) r_{sj} \Big|_0^H - c^* K_{zzsj} \frac{\partial r_{sj}}{\partial z}\Big|_0^H$$

$$\left. + \int_0^H G_{sj}\, dz + \int_0^H Q_{sj} dz \right\} \qquad (22)$$

One now assumes:

1. There is no diffusive transport through the top or bottom of the module domain. This assumption would not be valid if dry deposition were included in the RSM. Dry deposition is treated in RADM (through another module) instead.

2. There are no precipitation-borne pollutants falling into the top of the model (though physical situations can be easily imagined where this does occur, i.e., ice crystal seeding by high cirriform clouds or pollutants entering the upper troposphere). At the ground, $c^* w_{fsj} r_{sj}$ represents the wet deposition of pollutants.

3. $W_{aj}(z=H) = W_{aj}(z=0) = 0$ (air speed at module top and model bottom is zero).

4. The total mass in an operator cloud will be a summation over all species (indicated by index "s"). Performing this summation and including a stochiometric correction factor, m_s,

$$\sum_s m_s \int_0^{\delta t} dt \int_0^H G_{sj}\, dz = 0 \qquad (23)$$

Defining

$$f_b(0) = c^* w_{fsj} r_{sj} \qquad (24)$$

and

$$\vartheta = \int_0^H \frac{1}{A_j} \sum_{j \neq m} (F_{jm} r_{sj} - F_{mj} r_{sm})\, dz \quad , \tag{25}$$

then

$$M(t=\delta t) - M(t=0) = \int_0^{\delta t} dt\, [\vartheta + f_b(0)] \tag{26}$$

Within any one cell of the RSM, the change in mass is the time integral of mass removed from the bottom, and the mass brought in from the sides. Bookkeeping for these expressions is performed in SUBROUTINE DELTA_MASS.

2.5 AQUEOUS PHASE CHEMISTRY

The chemical species currently treated in the RSM include 1) the major ions found in eastern U.S. precipitation[1], (SO_4^{2-} NO_3^-, H^+, NH_4^+, and other cations), and 2) those species involved in the dominant SO2 aqueous oxidation pathways (SO_2, HOOH and O_3)[2]. The species and their forms (gas, aerosol, cloudborne, rainborne or snowborne) are summarized below:

- SO_2 gas, aqueous S(IV);
- sulfate aerosol, aqueous SO_4^{2-};
- nitric acid, nitrate aerosol, aqueous NO_3^-;
- ammonia, ammonium aerosol, aqueous NH_4^+;
- crustal cation aerosol, aqueous cation (this is treated as a lumped monovalent cation and essentially equals $2*[Ca^{2+} + Mg^{2+}]$);
- hydrogen peroxide gas and aqueous HOOH;
- ozone gas and aqueous O_3;
- H^+ in cloud and rain water; and
- aqueous CO_2 (aqueous concentrations are calculated based on equilibrium with 350 ppm CO_2 gas).

---

[1] Sea-salt components Na^+ and Cl^- are not included in the current RSM.
[2] As requested by Walcek, C. 1986a. Private correspondence (January 6, 1986).

The CO_2 species are not carried as dependent variables but their effects on H^+ are included in the aqueous chemistry routines.

As in PLUVIUS I MOD 5.0 code, the RSM distinguishes between "computed" and "constrained" species. The computed species are evaluated by explicitly taking into account transport, generation and decay (i.e., the RSM solves a conservation equation for each of them). The constrained species can be evaluated at any time from the values of the computed species, based on equilibrium or steady-state considerations. For more details on this scheme of categorization, the reader is referred to Easter and Hales (1984). The computed variables for each pollutant in the current RSM are:

- SO_2
  - gas + S(IV) in cloud water
  - S(IV), rainborne
  - S(IV), snowborne
- HOOH
  - gas + cloud
  - rainborne
  - snowborne
- sulfate
  - nucleating aerosol + cloud
  - non-nucleating aerosol[1]
  - rainborne
  - snowborne
- cation - same as sulfate
- nitrate
  - gas + cloudborne + nucleating aerosol[2]
  - non-nucleating aerosol
  - rainborne
  - snowborne
- ammonium - same as nitrate

---

[1]Aerosols are partitioned between nucleating and non-nucleating categories. The former is based on an assumed nucleation scavenging efficiency. In cloudy air, nucleating aerosol is assumed to be immediately incorporated into cloud water).

[2]In cloudy air, this is gas (HNO_3) and nitrate in cloud water (partitioned by solubility equilibrium). In cloud free air, this is gas and nitrate aerosol. At the moment this is arbitrarily partitioned; subsequent versions of the RSM will include the HNO_3 - NH_3 - aerosol equilibrium.

The lumping of different forms of a species may seem unusual. The species are grouped in this manner, however, to facilitate treatment of nucleation scavenging and the partitioning of soluble gases as equilibrium processes. Interactions diagrams illustrating the transfer processes included in the RSM are shown in Figure 4 - Figure 9. The following types of transfer processes are included:

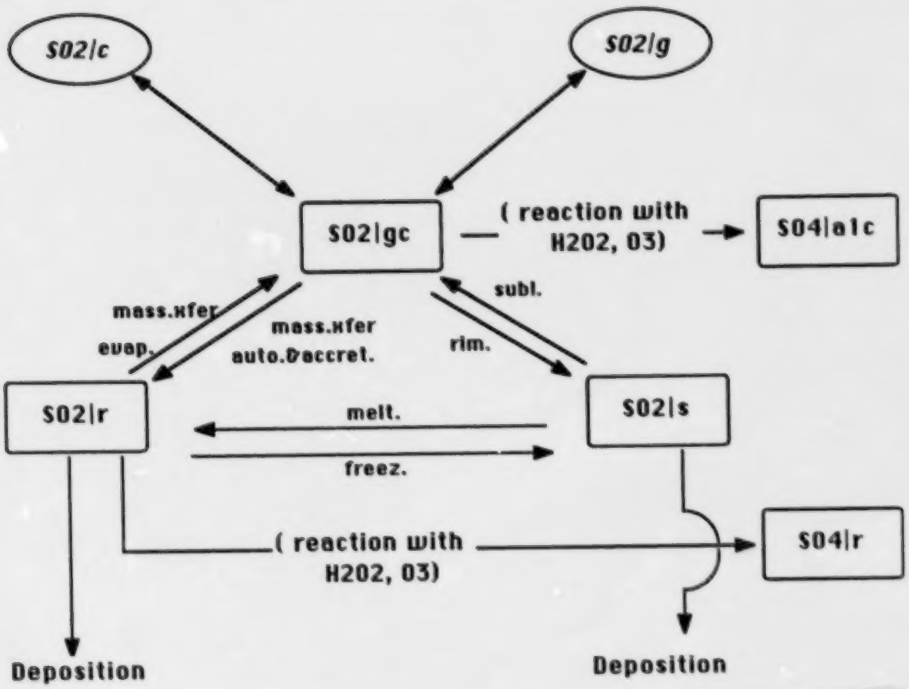
1. transfer between gas/aerosol forms and cloud/precipitation forms,

2. transfer between different cloud/precipitation forms by cloud processes, and

3. transfer from a chemical form to another form by aqueous-phase reactions.

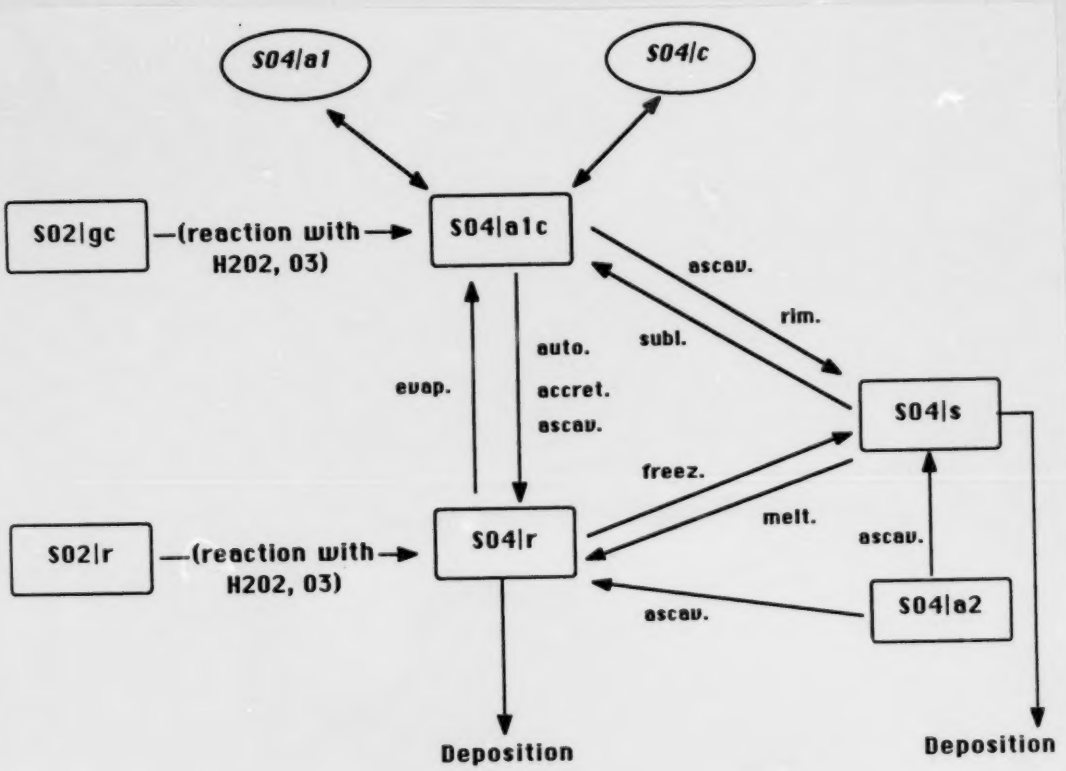
A list of the species names and associated mnemonic abbreviations for their phase (gas, aerosol, cloud, rain or snow) are given in Appendix B.

Solubility and dissociation parameters used in the RSM are based on the references in Appendix A, prepared by E. G. Chapman of Pacific Northwest Laboratory.



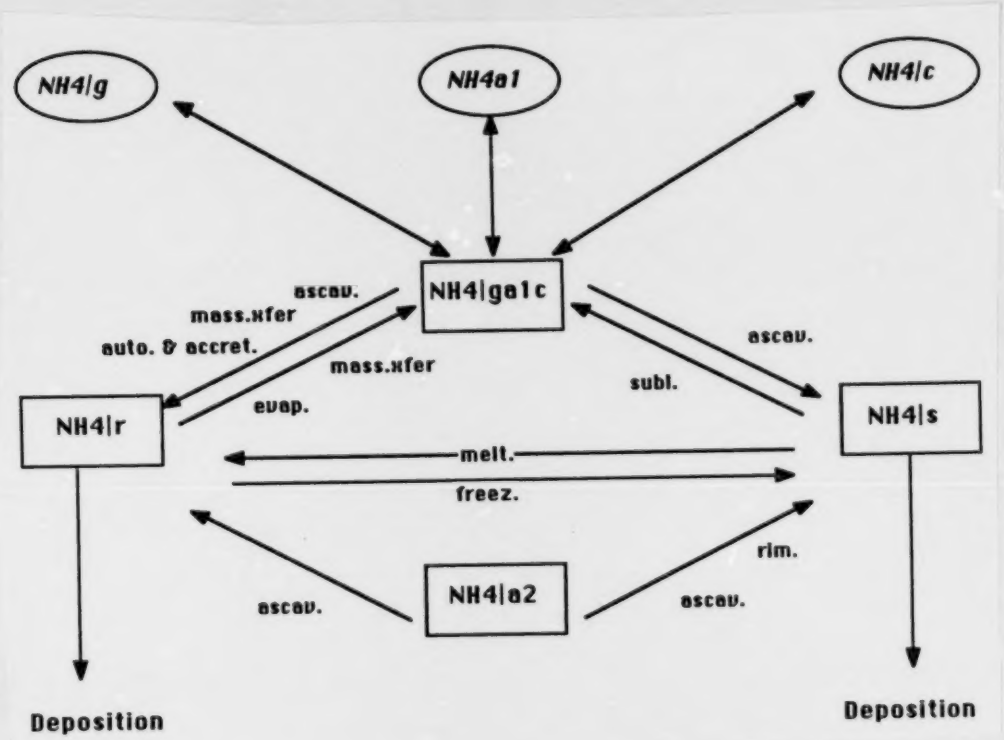
⟷	= a computed/constrained variable relation
→	= a transfer process between two computed variables
mass.xfer	= mass transfer between gas and rain phase
evap.	= evaporation
auto.	= autoconversion
accret.	= accretion
rim.	= riming
subl.	= sublimation
melt.	= melting
freez.	= freezing
ascav.	= aerosol scavenging by rain and snow (i.e., Brownian diffusion and inertial impaction)

Figure 4. Interaction diagram for SO_2.



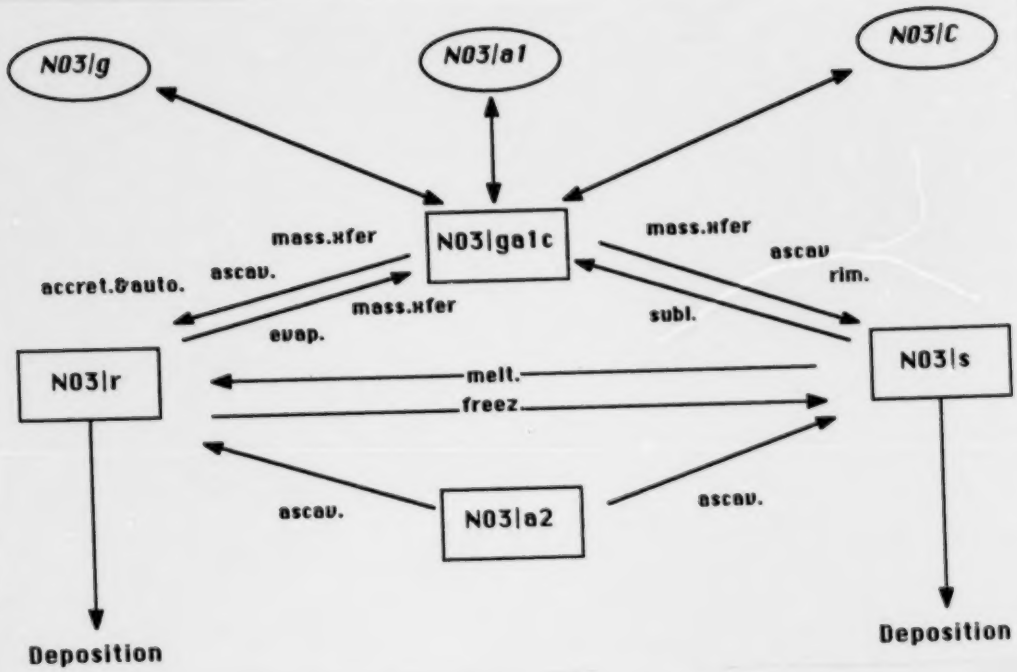
⟷	= a computed/constrained variable relation
⟶	= a transfer process between two computed variables
mass.xfer	= mass transfer between gas and rain phase
evap.	= evaporation
auto.	= autoconversion
accret.	= accretion
rim.	= riming
subl.	= sublimation
melt.	= melting
freez.	= freezing
ascav.	= aerosol scavenging by rain and snow (i.e., Brownian diffusion and inertial impaction)

Figure 5. Interaction diagram for SO_4^{2-}.



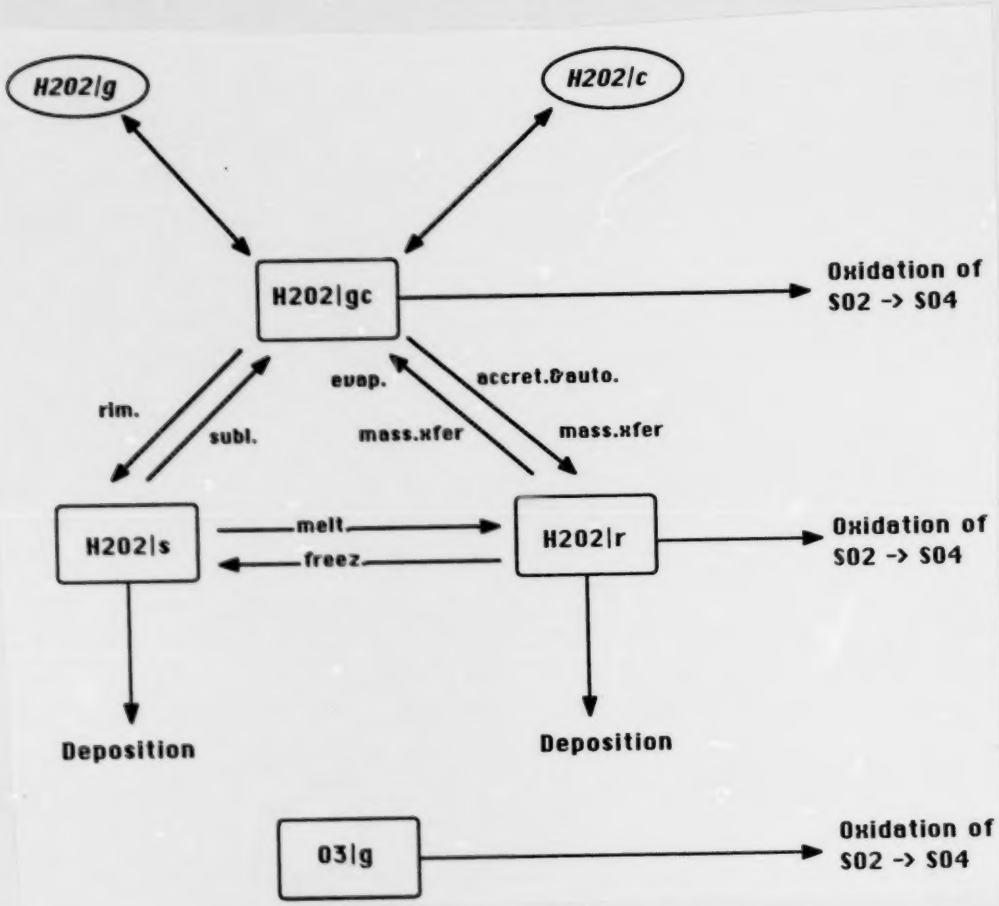
⟷	= a computed/constrained variable relation
→	= a transfer process between two computed variables
mass.xfer	= mass transfer between gas and rain phase
evap.	= evaporation
auto.	= autoconversion
accret.	= accretion
rim.	= riming
subl.	= sublimation
melt.	= melting
freez.	= freezing
ascav.	= aerosol scavenging by rain and snow (i.e., Brownian diffusion and inertial impaction)

Figure 6. Interaction diagram for NH_4.



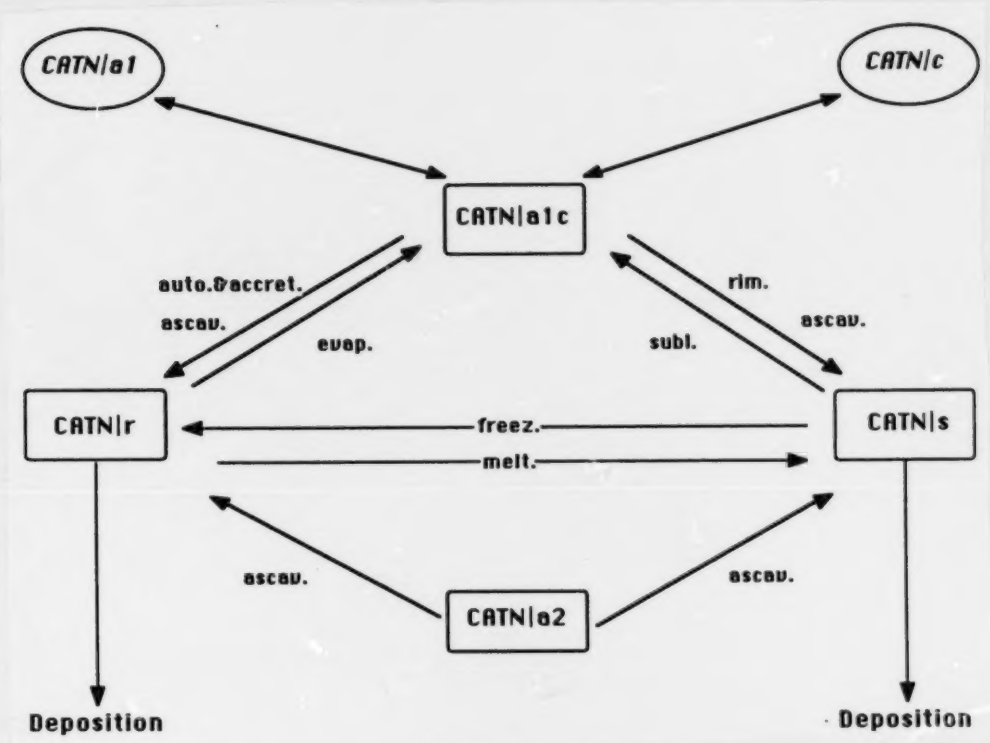
⟷	= a computed/constrained variable relation
⟶	= a transfer processes between two computed variables
mass.xfer	= mass transfer between gas and rain phase
evap.	= evaporation
auto.	= autoconversion
accret.	= accretion
rim.	= riming
subl.	= sublimation
melt.	= melting
freez.	= freezing
ascav.	= aerosol scavenging by rain and snow (i.e., Brownian diffusion and inertial impaction)

Figure 7. Interaction diagram for Nitrate ion and HNO_3 gas.



⟷	= a computed/constrained variable relation
⟶	= a transfer process between two computed variables
mass.xfer	= mass transfer between gas and rain phase
evap.	= evaporation
auto.	= autoconversion
accret.	= accretion
rim.	= riming
subl.	= sublimation
melt.	= melting
freez.	= freezing
ascav.	= aerosol scavenging by rain and snow (i.e., Brownian diffusion and inertial impaction)

Figure 8. Interaction diagram for HOOH and O_3.



⟷	= a computed/constrained variable relation
⟶	= a transfer process between two computed variables
mass.xfer	= mass transfer between gas and rain phase
evap.	= evaporation
auto.	= autoconversion
accret.	= accretion
rim.	= riming
subl.	= sublimation
melt.	= melting
freez.	= freezing
ascav.	= aerosol scavenging by rain and snow (i.e., Brownian diffusion and inertial impaction)

Figure 9. Interaction diagram for cation species.

2.6 INITIALIZATION OF AQUEOUS CHEMISTRY

Because the RADM does not carry aqueous-phase pollutants and the RSM does not "remember" such concentrations from the previous hour, an efficient initialization scheme for these species is needed.

This initialization is performed in four steps.

Step 1. Concentrations in cloud water are calculated based on nucleation scavenging of the initial aerosol and equilibrium solubilities of initial gases. These calculations are done in Subroutine AQEQUI (called from Subroutine GEN). The references in Appendix A describe the solubility coefficients. Pollutant mass is conserved in this step.

Step 2. Concentrations in precipitation are calculated assuming a simplified form of the conservation equation for species s carried in precipitation. For the stratiform region, this simplified form was derived by assuming

1. The only transport term arises from the fall speed of the precipitation w_f. This assumption is valid only in the stratiform region, where fall speeds are generally greater than the updraft (this will not be an assumption used in initialization of precipitation water in the convective storm region[1])

2. $$\frac{\partial c_s}{\partial t} = 0 \quad . \qquad \text{(i.e., a quasi-steady state exists)} \qquad (27)$$

---

[1] An analogous method is under development for the convective storm region, which will use conservation equations of the form:

for the updraft (column 2)

$$\frac{\partial}{\partial z} \left[(w_a + w_{fs}) c_{s,precip} \right] = - \dot{F}_{23} c_{s,precip} + S c_{s,cloud} \quad .$$

for the down draft (column 3)

$$\frac{\partial}{\partial z} \left[(w_a + w_{fs}) c_{s,precip} \right] = \dot{F}_{23} c_{s,precip} - \dot{F}_{3} \cdot c_{s,precip} \quad .$$

where $\hat{F} = F + Q$ (for definition of these terms, see page 6, "RSM Governing Equations").

3. The only source term, G, is associated with physical scavenging by cloud processes. Within any layer, this term can be approximated by the scavenging rate, S, (accretion or riming, depending on temperature) within the precipitation regime at height z'. These values are estimated from Scott's microphysical parameterizations.

These assumptions give:

$$\frac{\partial c_{s,precip}}{\partial t} = 0 = - \frac{\partial (w_{fs} c_{s,precip})}{\partial z} + S c_{s,cloud} \qquad (28)$$

Assuming "clean snow" at the operator cloud top (H) gives

$$c_{s,precip}\Big|_z = \frac{1}{w_{fs}\Big|_z} \int_z^H dz' \, S c_{s,cloud} \qquad (29)$$

By noting that

$$-(c_{s,precip} w_{fs})\Big|_z = \int_z^H dz' \, S c_{s,cloud}$$

$$= \int_{z+\Delta z}^H dz' \, S c_{s,cloud} + \int_z^{z+\Delta z} dz' \, S c_{s,cloud} \qquad (30)$$

$$= -(c_{s,precip} w_{fs})\Big|_{z+\Delta z} + \overline{S c_{s,cloud}}\Big|_z \Delta z \qquad (31)$$

where

$$\overline{S c_{s,cloud}} = \frac{1}{2}\left[(S c_{s,cloud})\Big|_{z+\Delta z} + (S c_{s,cloud})\Big|_z \right] \qquad (32)$$

the following algorithm is obtained for estimating the precipitation concentration of pollutant "s" at height index "k" within the stratiform region

$$\left(C_{s,precip}\right)\Big|_k = -\frac{1}{\left(w_{fs}\right)\Big|_k}\left[-\left(C_{s,precip}w_{fs}\right)\Big|_{k+1} + \left(S\,C_{s,cloud}\right)\Big|_k \Delta z\right] \quad . \tag{33}$$

This second step does not conserve pollutant mass; pollutant placed in precipitation is not balanced by a reduction of cloudborne pollutant.

Step 3. Cloud and precipitation-borne pollutant concentrations are adjusted to conserve mass. Adjusted concentrations are defined by

$$C'_{s,cloud} = \alpha_s C_{s,cloud} \quad , \tag{34}$$

$$C'_{s,precip} = \alpha_s C_{s,precip} \quad , \tag{35}$$

where α_s is chosen so that

$$\alpha_s \int_0^H \left(C'_{s,cloud} + C'_{s,precip}\right) dz = \int_0^H C'_{s,cloud}\, dz \quad . \tag{36}$$

(i.e., the total waterborne pollutant mass after Step 3 equals the total waterborne pollutant mass after Step 1). This results in

$$\alpha_s = \frac{\int_0^H C_{s,cloud}\, dz}{\int_0^H \left(C_{s,cloud} + C_{s,precip}\right) dz} \tag{37}$$

Step 4. The final step in initilizing the precipitation-borne concentrations is a two-fold process of 1) redefining the constrained species and 2) adjusting the gas and cloudborne species concentration to be in chemical equilibrium. Redefinition of constrained species is necessary so that the "lumped" species (i.e., sulfate aerosol available for cloud nucleation and sulfate in cloud water) are indeed the sum of their constrained equivalents.

By way of example, the updated value of the concentration of aerosol plus cloudborne sulfate in RSM cell (i,j,k), C(I,J,K,KSO4A1C), is redefined to be

C(I,J,K, KSO4A1C) = C(I,J,K, KSO4A1) + C(I,J,K, KSO4C)

Finally, chemical equilibrium between gas and cloudborne species is computed using the solubility algorithms first employed in Step 1 of the precipitation-chemistry initialization.

SECTION 3

CODE CHARACTERISTICS--AN OVERVIEW

Although the aqueous-phase chemistry is time dependent, the cloud features and the ambient pollution fields in each of the operator clouds of the RSM are assumed to be in a steady state. This assumption was necessitated by the one hour simulation time interval between calls from the host code to the scavenging module. This interval was not felt to be adequate to generate a realistic cloud environment using a time-dependent model. Concerns about excessive computer usage were a secondary reason for not using the more realistic time dependent approach.

As indicated previously in section 2.2, the four "cells" (or operator clouds) available in the RSM can be used to simulate three types of cloud environments. Cell 4 can be used for the downdraft of a nonprecipitating cumulus. Cells 2 and 3 can be allocated to the updraft and downdraft region of a convective storm system. Cell 1 can be used for a) a widespread precipitating stratiform environment, b) the updraft of a non precipitating cumulus, or c) a clear air buffer region when only convection but no stratiform cloud exists. Such a clear air buffer zone is necessary to account for subsidence circulations outside the convective storms or clouds.

3.1 STRATIFORM PRECIPITATION (cell 1)

These regions are characterized by relatively small updrafts (<15 cm/s) covering most of the horizontal area of the grid column. Calculations of cloud characteristics within these zones are based on the RADM/MM4 provided profile of vertical velocity. The storm model of Scott (1986a) is applied with an updraft based on a smoothed form of the RADM/MM4 supplied updraft, as described in section 2.3.

The code outlined by Scott (1986a)[1] is designed to provide an updraft and cloud parameters consistent with a specified precipitation rate. This feature was incorporated into an earlier version of the RSM. It was removed because it would have introduced a second large scale motion to the field

[1]Scott, B. C. 1986a. "User's Manual for the Cloud and Scavenging Module." (In preparation.)

already defined by MM4 and used in RADM. Thus, there would be the potential for vertical transport being calculated once by RADM and a second time by the RSM. A further complication to this earlier approach was the artificial generation of mass that would have been introduced into the RADM system by having an updraft that was not in dynamic balance with the surrounding RADM grids. Only those subroutines described by Scott that calculate the cloud parameters for a given updraft are used in the RSM. No use is made of the provision to adjust the updraft profile to produce a specified precipitation rate.

If the RADM/MM4 updraft profile (Eq. 19), in conjunction with the Scott microphysics, results in a precipitation rate greater than a specified critical amount (presently set at 0.01 mm/hr), the resulting cloud is used to define a scavenging environment (cloud and precipitation water, riming/accretion/evaporation rates) in which time-dependent scavenging and aqueous chemistry calculations are performed. If the resulting precipitation rate is less than this critical value, the potential for fair weather cumulus is examined.

In the current stratiform model, only two water categories are used: cloud water and precipitation. The crude vertical resolution in the vicinity of the freezing level does not justify the inclusion of precipitation melting and freezing (these are treated as occurring instantaneously).

Cloud water is assumed to move with the air velocity, in contrast to precipitation water, which falls with respect to the air. Precipitation is parameterized with a Marshall-Palmer size distribution. The fall speeds and cloud-water collection rates for precipitation depend on the classification of precipitation as snow or rain, which, in turn, depends upon the local air temperature (defined by a moist adiabatic profile from cloud base).

Precipitation embryos are assumed to be ice crystals, which grow at the top of the cloud by vapor deposition until they reach dimensions of 400 μm. Growth then continues by vapor deposition and accretion as the crystals fall. Below the freezing level, the ice particles melt, accelerate, continue to accrete cloud droplets, and fall to the surface as millimeter size rain drops.

Within the model domain, the water concentrations are determined by a balance between the liquid water produced in a region, the water passing in or out through the boundaries of the region, and the water removed from the

region after capture by falling precipitation. Specifically, by denoting M_c and M_p as the mass of water per unit volume of space associated with cloud water and precipitation water, respectively, the local change of each quantity within a precipitating cloud is given by

$$\frac{\partial M_c}{\partial t} = -\nabla_H \cdot (V_H M_c) - \frac{\partial}{\partial z}(w_a M_c) + D_c - C_p \quad . \tag{38}$$

$$\frac{\partial M_p}{\partial t} = -\nabla_H \cdot (V_H M_p) - \frac{\partial}{\partial z}((w_a + w_{fp}) M_p) + D_p + C_p \quad . \tag{39}$$

where V represents the wind velocity vector and w_{fp} the fall speed of precipitation. D represents the rate diffusion of moisture from the air to cloud or precipitation water and C represents the collection of cloud water by precipitation.

These equations are solved in a steady-state, one-dimensional form to obtain pertinent profiles of M_c and M_p every time the stratiform cloud is activated. The horizontal divergence term,

$$\nabla_H \cdot (V_H M) \quad , \tag{40}$$

is treated as in the RSM main conservation equations and results in a horizontal inflow/outflow to the stratiform cell. Outflow depletes the M_c and M_p; inflow air is assumed to have $M_c = M_p = 0$. The horizontal transport is related to the stratiform updraft through the continuity equation for air,

$$\nabla_H \cdot (c^* V_H) + \frac{\partial}{\partial z}(c^* w_a) = 0 \quad . \tag{41}$$

but there is still considerable freedom in specifying V_h. Currently this freedom is used to adjust V_h to obtain a desired storm efficiency, E, defined as

$$E = \frac{\text{surface precipitation flux}}{\text{inflow vapor flux}}$$

It should be noted that since M_c and M_p are calculated only within the RSM (and not in dry-RADM), all transport terms in the above equations must be computed by the RSM. This procedure differs from the way in which dry-RADM computes such transport for pollutant species.

3.2 CONVECTIVE PRECIPITATION (cells 2 [updraft] and 3 [downdraft])

These regions are characterized by relatively large vertical velocities (>1 m/s) occupying small fractional areas. The precipitating convective clouds is simulated with adjacent updraft and rainshaft (or downdraft) cells. Currently, the two cells are assumed to occupy a constant fractional area of the grid-column. In the updraft cell, cloud and precipitation water are assumed to move upward or to be suspended by the updraft. When the water concentrations in the updraft portion exceed a prespecified threshold value, the excess water is transferred to the rainshaft cell. The precipitation in the rainshaft cell then falls out through a saturated downdraft. Both cells are assumed to be in steady state. The updrafts and downdrafts are adjusted so that the precipitation in the downdraft cell matches the convective precipitation specified by the RADM/MM4 code. The results from a series of computations using this model have been combined into a lookup table. When the precipitating convective cloud is activated by the RSM, the cloud environment within the two cells is obtained by interpolation of the lookup-table values.

3.3 NONPRECIPITATING CUMULUS (cells 1 [updraft] and 4 [downdraft])

The non-precipitating cloud model of Ritter and Stedman (1985) is being modified by Vukovich (1986)[1] for inclusion into the RSM. This set of subroutines will be used in the absence of stratiform clouds when the host-provided temperature and moisture profiles result in a heat and moisture convergence adequate to generate a field of fair weather cumulus. Venting induced by cumulus may play a major role in vertical transport and these clouds may also have a major effect on photochemistry via their role as obscurants to insolation. There is also evidence that fair weather cumulus clouds greatly increase the effective oxidation rate of many species as a result of their rapid condensation/evaporation cycles.

3.4 LOGICAL FLOW: AN OVERVIEW

This section contains an overview of the subroutine calling sequence within the RSM. This calling sequence is illustrated in Table 2. The modular nature of the RSM allows the user to modify those components that he feels can be improved upon with minimal modification to the rest of the

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[1]Vukovich, F. 1986. "User's Guide to CUVENT." (In preparation.)

code. To aid in presentation of the overview of the calling sequence, only those subroutines shown in the following outline will be discussed (a more complete outline is contained in section 3.6). As described in Table 2, a subroutine positioned with N levels of indentation is called by the preceding subroutine with only N-1 levels.

A listing of the subroutines that make up the RSM will be published in a future report. The user should refer to Appendix C for a description of the subroutines.

The format for the calling sequence of the RSM from the RADM host code has not yet been finalized. However, based on discussions with the NCAR modeling team, the RSM has been designed on the assumption that the RADM will specify the (i,j) coordinates at which scavenging and aqueous phase calculations are to be performed.

TABLE 2. SUBROUTINE CALLING SEQUENCE: OVERVIEW

```
Host code calls RSM:
SUBROUTINE RSM
   if initial call from RSM:
   (Read(9,*) KDIAG_OLD, TRANS, KRSCAV, KNRSCAV,KYINTEG)
   CALL BLOCKDATA:          define parameters, arrays, data statements
   CALL INPUT1              define control variables
   CALL GRDXYZ              define RSM grid (12 km, 20 layer)
   ------------------------------------------------------------------
   at start of each call from RADM:
   CALL INPUTMET            definition of meteorological environment
      CALL INPUT_MM4        read data from MM4 files: define z(σ)
         CALL READMET:      read synoptic files from MM4
   for each RADM grid:
      CALL MM4_TO_RSM       interpolate MM4 values to RSM grid
      CALL CLOUD_BASE       calculate cloud base from MM4 temp.
   if convective precipitation:
   CALL CONVCLD_TOP         estimate convective cloud top
   CALL CLOUD_CONV          define convective cloud
   CALL CLOUD_TOP           define stratiform cloud top
   CALL CLOUD_STRATI        define stratiform cloud
   if precip. rate <0.01 mm/hr:
   CALL CUVENT              define fair weather cumulus.
CALL GRDSET                 define grid expansion factors
CALL INIT                   initialize chemistry values
   CALL INPUT_RADM          get clear air values from RADM
   CALL RAIN_INIT           initialize aqueous phase chemistry
repeated calls to:
CALL CORE                   numerical integration
```

In the present form, the RSM structure has been designed to be activated by RADM at appropriate simulation times and, at these times, to analyze the scavenging processes over many grids. SUBROUTINE RSM is the governing routine for controlling the many modules that accomplish this action.

SUBROUTINE RSM begins by reading two data files. Logical unit 9 ("DIAG.DAT," or FOR009 in VMS control language) contains variables that act as flags, which activate or deactivate algorithms related to a) the printing of key values, b) reactive scavenging, c) cloud transfer processes and d) horizontal flux terms. These variables are intended for user modification. Details of how they may be modified are given in section 4. The second file (logical unit LUNIN, FOR021 = "INPUT.DAT") is read in SUBROUTINE INPUT1; it contains many of the control variables that are the same for all simulations. This second file is not intended for user modification.

Definition of the RSM grid is performed in SUBROUTINE GRDXYZ. It is presently set to define a 20-layer vertical grid structure with top at 12 Km. Because a geometrical height system is used throughout the RSM and because RADM employs a sigma coordinate system, an interpolation routine is necessary when using the RADM values in the RSM. SUBROUTINE INPUT_MM4 assigns height values to the sigma system via the following algorithm:

1. The RADM sigma values are converted to pressure p, from the relation:

$$\text{sigma} = \frac{p - p(\text{top})}{p(\text{sfc}) - p(\text{top})} .$$

2. The temperatures at these sigma values are used to define a mean column temperature, <T>.

3. The hydrostatic equation is integrated upward from the ground to define a corresponding height coordinate at a given sigma level:

$$z_{\text{upper}} = z_{\text{lower}} - \frac{R\ \langle T \rangle}{g} \ln(p_{\text{upper}}\ p_{\text{lower}})$$

where R and g are the gas constant for dry air and the acceleration of gravity, respectively.

SUBROUTINE INPUT_MM4 also calls the host-code provided subroutine and reads the synoptic format data from MM4 (SUBROUTINE READMET); this subroutine is called only at the start of each call to the RSM.

Having loaded RADM/MM4 values into the RSM and identified their height, SUBROUTINE MM4_TO_RSM then interpolates those variables from the RADM grid to the RSM grid. These interpolated values are necessary for checks on consistency between the the RSM and RADM values of moisture, updraft, pressure, and temperature. The interpolation algorithm used to estimate or define any RADM variable X, at a given geometrical height between the associated values defined at fixed sigma layers of MM4 is

$$X(z) = X_{lower} + a \ln(p/p_{lower}),$$

where

$$a = \frac{X_{upper} - X_{lower}}{\ln(p_{upper}/p_{lower})}$$

and

$X(z)$ is the interpolated quantity at height z,

X_{lower} is the value of X at the lower sigma level,

X_{upper} is the value of X at the upper sigma level,

p is the pressure at the geometric height of interest estimated from $p = p_{lower}\exp(-g\ DZ/R\ \langle T \rangle)$, where $DZ = Z - Z\ (\sigma_{lower})$

p_{upper} is the pressure value associated with the upper sigma coordinate, and

p_{lower} is the pressure value associated with the lower sigma coordinate.

This scheme produces the same values that would be estimated by a straight line interpolation between pressure heights plotted on Skew-T Log p chart; as such, it lends itself to easy quality-assurance checks by simply plotting the values on these common graphs.

SUBROUTINE CLOUD_BASE uses the lifting condensation level calculated from surface conditions to define the height of cloud base in all the RSM subgrids. For the situation where MM4 specifies convective precipitation at

a given grid, a cloud top for the convective system is defined by determining the level of neutral buoyancy for a surface air parcel lifted along a moist adiabat. SUBROUTINE CONVCLD_TOP evaluates T',

$$T' = T_0 + \int_{p_0}^{p} \left.\frac{dT}{dp}\right|_{moist} dp' \qquad (42)$$

up to the pressure level where T' is equal to the environmental temperature. If this level of neutral buoyancy cannot be found, then the convective cloud top is defined to be 12 Km. With the convective storm precipitation rate defined from MM4 and estimates of cloud base and cloud top calculated, the convective-storm lookup tables are accessed and a corresponding scavenging environment for cells 2 and 3 is computed. This scavenging environment is defined by vertical profiles of

1. updraft speed,
2. cloud and precipitation water,
3. particle fall speeds,
4. the flux into and out of each cell,
5. scavenging rates (accretion or riming) and
6. the mass of precipitation falling from the updraft to the rainshaft cell.

Development of a stratiform-cloud scavenging environment is initiated in CLOUD_TOP. This subroutine defines the thickness and updraft profile of the stratiform layer (see also section 2.3). This information goes to SUBROUTINE CLOUD_STRATI to define the scavenging environment for RSM cell 1.

If no precipitation is predicted by Scott's microphysical model, then SUBROUTINE CUVENT is called to either define a region of fair-weather cumulus or to determine that such clouds do not exist. If no clouds exist whatsoever, then analysis of scavenging calculations are terminated at this grid and the RSM begins analysis of an adjacent RADM grid.

If any operator clouds have been defined, then SUBROUTINE INIT specifies the initial profiles of pollutant species in each RSM cell. First, SUBROUTINE INPUT_RADM defines the profiles of clear-air pollutant species.

Currently this routine sets up some arbitrary profiles for testing purposes. Eventually this routine will take RADM profiles of clear-air species and interpolate them to the RSM vertical grid. Next SUBROUTINE RAIN_INIT uses the algorithms defined in section 2.6, to evaluate the associated rain/snow water concentrations.

This completes the initialization portion of the RSM. The next step is to integrate the conservation equations for pollutant species (Eq. 15) over the one hour time period. This is performed by repeated calls to SUBROUTINE CORE.

3.5 DATA INPUT

Only two input data sets are expected to be modified by the user. The first set consists of the variables KDIAG_OLD, KRSCAV, KNRSCAV, and KYINTEG. These variables are read from file DIAG.DAT. Their values and roles are discussed in section 4. No other variables from LUNIN are intended for modification.

Meteorological data for the RSM is presently read from file FOR026 by Subroutine READMET. This subroutine was designed to simulate the transfer of meteorological data from the RADM/MM4 system to the RSM. The actual transfer procedure cannot be finalized until the RSM is included into the host code.

Data from RADM/MM4 has been presented in synoptic format, where data blocks are partitioned by time, with each data block containing meteorological data at all host-code grid points. A data block is read at the start of each RSM simulation. In its present form, the RSM uses only data within the block that applies to those grids defined in "Program RADM", a short test code designed to simulate the RADM computing environment. "Program RADM" loops through several grids, the meteorological conditions of which have been defined by the first call to READMET.

The following documentation of the input data routine and the data themselves are based on Walcek.[1] The data set covers a 3 x 17 horizontal domain with 15 vertical layers. READMET loops over the east-west (IMAXMM4) direction and over the north-south (JMAXMM4) within DO loop 10 of Subroutine READMET:

```
DO 10  I = 1, IMAXMM4
DO 10  J = 1, JMAXMM4
```

[1] Walcek, C. 1986b. Private correspondence (May 2, 1986).

The following READ statements are performed for each I,J combination:

1. READ(26,*,END=998) IT, II,IJ, TSF, PSURF(I,J), RTOTARRAY(I,J), RCONVARRAY(I,J), ELEVARRAY(I,J),

   where IT is the time (GMT) (22, 23 or 24 for April 1981),

   II is the east-west "I" index (see map 1 for location),

   IJ is the north-south "J" index (see map 1 for location),

   TSF is the surface temperature (K),

   PSURF(I,J) is the surface pressure (mb),

   RTOTARRAY(I,J) is the total rain in previous hour (cm),

   RCONVARRAY(I,J) is the convective rain in the previous hour (cm), and

   ELEVARRAY(I,J) is the surface elevation.

2. READ(26,*) (TARRAY(I,J,K), K = 1, KMAXMM4),

   where TARRAY(I,J,K) is the temperature (K) at grid coordinate (I,J,K).

3. READ(26,*) (URRAY(I,J,K), K =1, KMAXMM4)

   where URRAY(I,J,K) is the east - west wind (m/s) at grid coordinate (I,J,K).

4. READ(26,*) (VARRAY(I,J,K), K=1, KMAXMM4),

   where VARRAY(I,J,K) is the north-south wind (m/s) at grid coordinate (I,J,K).

5. READ(5,*) (QARRAY(I,J,K), K = 1, KMAXMM4)

   where: QARRAY(I,J,K) is the water vapor mixing (g/kg) ratio at grid coordinate (I,J,K).

The calculations in the DO 20 loop compute vertical velocity using UARRAY and VARRAY values from adjacent grid squares. This algorithm was provided to PNL by NCAR. All vertical velocities are computed at the full sigma levels by using a mass continuity equation.

3.6 MODULAR CONSTRUCTION

Table 3 contains an outline that illustrates the calling sequence between subroutines in the RSM. Entries in the outline refer to subroutines of the RSM. In this outline:

1. A subroutine positioned with N levels of indentation is called by the preceding subroutine with only N-1 levels. By way of example, if Program Main called Subroutine SUB1 which in turn called Subroutine SUB2, the outline entry would be as follows:
   MAIN
       SUB1
           SUB2

2. Subroutines with (strati.) after them are documented in Scott (1986a). These are subroutines involved with microphysical definition of the stratiform region.

3. Subroutines with (Pluv1) after are them are documented in Easter and Hales (1984). These are subroutines based on earlier work with PLUVIUS MOD 5.0 They are involved with integration of the equations describing chemistry. They also include several utility routines (e.g., calculation of vapor pressure).

4. Subroutines marked with (Pluv2) are subroutines under development for use in PLUVIUS II. They are primarily the integration routines involved with vertical transport.

5. Subroutines with (conv.) are being documented by Scott (1986b).[1] These are subroutines involved with the microphysical definition of the convective storm regions.

6. Subroutines with no post-script identification are described in Appendix C. A glossary in Appendix B defines key terms from this category of subroutines.

7. Subroutine CUVENT will be documented by Vukovich.[2]

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[1]Scott, B. C. 1986b. "User's Manual for the Convective Storm Component of the RSM." (In preparation.)
[2]Vukovich, F. 1986. "User's Guide to CUVENT." (In preparation.)

TABLE 3. SUBROUTINE CALLING SEQUENCE[1]

RSM called from host code:

- I. BLOCKDATA
- II. INPUT1
- III. GRDXYZ
- III. INPUTMET
  - A. INPUT_MM4
    - 1. READMET
    - 2. TPLOT
      - a. STABCLASS
  - B. CLOUD_BASE
    - 1. ESAT (Pluv1)
    - 2. TEMP_LIFTED_DRY
      - a. DTDPDRY
  - C. CONVCLD_TOP
    - 1. TEMP_LIFTED
      - a. DTDP
        - i. SAT (Pluv1)
  - D. CLOUD_CONV (conv.)
  - E. INIT_CONV
  - F. CLOUD_TOP
    - 1. RELHUM
    - 2. TEMP_LIFTED
  - G. GRDXYZ (Pluv1)
  - H. MM4_TO_ASM
  - I. CLOUD_STRATI
    - 1. SIGMA_BCS
      - a. RHOAIR (Pluv1)
      - b. RLAPSE (Pluv1)
    - 2. DEFAULT (strati.)
    - 3. DEFAULT (strati.)
    - 4. MAIN (strati.)
      - a. WINDS_BCS (strati.)
        - i. NEWTON (strati.)
      - b. WATER (strati.)
        - i. XMULT (strati.)
        - ii. COEF (strati.)
        - iii. VDEP (strati.)
        - iv. NEWTON (strati.)
      - d. DEFAULT (strati.)

[1]See text page 40.

TABLE 3. (continued)

J. INIT_STRATI
1. RHOAIR (Pluv1)
2. BLWCLOUD
3. ABVCLOUD
4. SAT (Pluv1)

K. CUVENT

V. GRDSET (Pluv2)

VI. INIT

A. INPUT_RADM

B. RAIN_INIT

1. CALLGEN

a. GEN (Pluv1. & Pluv2)

i. SAT (Pluv1)

ii. SSAT (Pluv1)

iii. MICRO

α SAT (Pluv1)

β SSAT (Pluv1)

iv. AQUPHA (Pluv2)

α DISSCON (Pluv2)

β AQEQUIL (Pluv2)

γ AQNONEQ4 (Pluv2)

v. SNOWFALV (Pluv2)

1. RIDIAG
2. THICK
3. SCAVCOEF
4. CALLGEN
(routines listed for previous call to CALLGEN follow as before)
5. RIDIAG

VII. METSUM

VIIX. CHEMSUM

IX. MASS_SUM

A. THICK

X. PRINTI (Pluv2)

XI. TIMESP (Pluv2)

XII. DATADUMP

XIII. CORE (Pluv2)

XIV. PRINT (Pluv2)

XV. METSUM

XVI. CHEMSUM

XVII. MASS_SUM

SECTION 4

USE OF DIAGNOSTIC FLAGS IN THE RSM

There are many processes being simulated in the RSM in time dependent chemical environments. During the development of the RSM, it was useful to run the code with selected processes "turned off." This greatly simplified analysis of the results, both for internal consistency and for consistency with results intuitively expected for these selected (ideal) conditions. Output from subroutine MASS_SUM was found to be the most useful in determining the performance of the RSM.

There are five variables read from file LUNIN which can be used for such diagnostic studies of the RSM.

Following is a summary of these flags and their effect on the RSM:

Flag Name	Value	Result
KDIAG_OLD	>0	Values of key variables in each subroutine printed to file FOR006
	<0	Values not printed
KRSCAV	>0	Reactive scavenging processes simulated (mass transfer and aqueous chemistry are included in this definition of reactive scavenging)
	<0	Reactive scavenging processes turned off
KNRSCAV	>0	Nonreactive scavenging processes simulated (cloud microphysical transfer processes)
	<0	Nonreactive scavenging processes turned off
KYINTEG	>0	Horizontal exchange calculated between RSM cells dynamic flux terms
	<0	No horizontal exchange between cells

KTRANS	>0	Vertical transport calculated
	<0	Vertical transport turned off

None of the above flags will effect the partitioning of species between computed and constrained species.

Using these flags, the following tests have been used as quality control checks against various processes in the RADM Scavenging module:

1. KRSCAV < 0, KNRSCAV < 0 and KTRANS < 0
   Should result in no changes relative to the initial values in any water-borne or air concentrations after a one-hour simulation.

2. KRSCAV < 0, KNRSCAV < 0 and KTRANS > 0
   With transport being the only process simulated in the RSM, there should be a decrease (relative to the initial conditions), in the rainborne and snowborne pollutants as they are removed at the bottom of the model. With the greater fallspeeds, rainborne pollutants should undergo a greater decrease in concentration than the corresponding snowborne pollutants. For short simulations (less than 10 minute simulation time), the decrease in snowborne pollutants (with their smaller fallspeeds) should be relatively "small" relative to rainborne pollutants. For longer simulations, the decrease of both should be comparable.

   Constrained variables are not transported and hence not removed at the lower boundary of the model; there should be no change in these species.

3. KRSCAV < 0, KNRSCAV < 0, KSCAV > 0, KTRANS < 0
   With only microphysical interactions between cloud, vapor and rain particles occurring, there should be an increase in the rain and snowborne pollutant levels with a corresponding decrease in the cloudborne pollutants (since the precipitation will be accreting or riming with the cloud particles).

4. KRSCAV > 0, KNRSCAV < 0, KTRANS < 0
   With only reactive scavenging occurring, there should be mass conservation within the following groups of computed species:

   a. nitrogen compounds = KNO3GA1C + KNO3A2 + KNO3R + KNO3S
   b. sulfur compounds = KSO2GC + KSO2S
   c. ammonia compounds = KNH4GA1C + KNH4A2 + KNH4R + KNH4S
   d. all computed variables taken together.

5. for any combination of diagnostic flags, the molar sum of the partitioned variables should equal the molar value of the associated constrained variables.

6. The solubility of sulfate and ammonia should result in cloud concentrations equal to a much larger value than the associated gas phase concentrations following the call to RAIN_INIT. The corresponding values for NO_3^- should be approximately equal.

SECTION 5

PROPOSED BENCHMARK TESTS: COMPARISON WITH PLUVIUS II

In a proposed benchmark test, a comparison will be made between the values of aqueous chemistry and deposited mass as predicted by the scavenging module and a closely related code, PLUVIUS II.

Many of the routines in the scavenging module were taken from PLUVIUS II. In a simplified way, the only difference between the two codes is that the scavenging module can initialize the cloud environments using only a meteorological temperature and moisture sounding from the host code.

To insure that no errors have been introduced into those routines which were taken from the PLUVIUS II, the following test is proposed:

a. The scavenging module will use data from the host code to define a complete set of initial conditions. These conditions will include updraft speeds, scavenging rates and cloud characteristics (cloud base, cloud top and profiles of cloud and precipitation water).

b. A set of clear air chemistry values will be used to initialize the aqueous phase chemistry.

c. These initial conditions will be used by the scavenging module for a one hour simulation of the chemistry and wet removal within the scavenging environment.

d. These same initial conditions will be used in the PLUVIUS II code.

If a series of such tests compare "favorably," then PNL will have established that the algorithms defined in the user's guide have been correctly implemented into the numerical integrator of the PLUVIUS II framework.

SECTION 6

LIMITATIONS OF THE RSM

In this section we present a summary of key assumptions within the RADM Scavenging Module. The user should be aware of these assumptions.

Issue 1. Precipitation Melting in Stratiform Cloud

The microphysical model of (Scott 1986a)[1] treats precipitation as a single species having the properties of either rain or snow, depending on the temperature. There is no region within this model where snow has fallen below the freezing level and rain and snow co-exist. This is equivalent to having assumed instantaneous melting of snow as it falls through the freezing level. In fact, melting is a slow enough process to allow for an extensive region of mixed snow and rain.

In the RSM, precipitation-borne pollutants are treated as two separate variables i.e., the rainborne and snowborne form. This requires that a melting rate for snow to rain (an snowborne and rainborne pollutants) be specified. Also, the fullspeed for rain and snow must be defined throughout the vertical domain. Setting the snowfall speed to zero, below the freezing level, results in undesirable numerical errors.

Subsequent versions of the RSM will resolve these problems by the addition of a finite melting rate into the basic stratiform model. For now, these difficulties have been resolved by:

1. defining a large melting rate for snow particles below the freezing level. This rate has somewhat arbitrarily been defined as 0.1/second. It has the effect of transferring all of the snowborne species into the corresponding rainborne elements within a few grids below the freezing level.

2. defining the fallspeed for snow or rain particles below or above the freezing level to have speeds equal to the respective values at

[1]Scott, B. C. 1986a. "User's Manual for the Cloud and Scavenging Module." (In preparation.)

the freezing level. This results in a small non-zero fall speed (typically 3 m/s) for rain particles above the zero degree isotherm and a fall speed of less than 1 cm/s for snow particles below. This produces a smooth profile of fall speeds which reduces the numerical errors associated with transport calculations.

Issue 2. Warm Cloud Processes

Precipitation in the stratiform model results from the nucleation of ice crystals which grow at the top of the cloud by vapor deposition and which fall out and grow by further deposition and accretion. This mechanism is not appropriate for cloud tops with temperatures above freezing.

In the present RSM, cloud top is forced to be at least at the freezing level. Future versions of the RSM will allow for warm cloud precipitation initialization mechanisms.

Issue 3. Steady State Convective Storms

The questionable reality of steady state convective storms is acknowledged. Given that the RADM/MM4 system

1. specifies only the cumulative convective precipitation amount,

2. does not carry cloud conditions from one simulation time call of the RSM to the next, and

3. provides only hourly soundings of temperature and moisture,

no alternative approach to developing a convective cloud environment was seen which would be feasible in terms of computer resources and the number of assumptions necessary for implementation. The steady state assumption also allowed a look-up table approach to be used in defining the scavenging environment, further reducing the demands on computer resources.

Issue 4. Definition of Cloud Top

The height of the stratiform cloud is central to definition of the stratiform environment (Scott, 1986a).[1] In specifying the height at which the stratiform cloud top occurs, use has been made of the simplest definition possible, namely, that cloud top occurs when the updraft is "small", which for the purposes of the work here, means less than 0.015 cm/s.

---

[1]Scott, B. C. 1986a. "User's Manual for the Cloud and Scavenging Module." (In preparation.)

Issue 2, "Warm Cloud Processors," has forced further modification to this definition of cloud top.

Issue 5. Area of Convection

The magnitude of the fractional area of convection will play a key role in defining the value of any variable within the the RSM grid. In the present version of the RSM, this key number has been set to 10% of the host grid area. This somewhat arbitrary number is based on data presented by Krishnamurti (1968) and Changnon (1981). Subsequent versions of the scavenging module will contain a more refined method of evaluating this value.

Issue 6. Storm Efficiency

The efficiency of the stratiform storm model is defined from u and v wind components, which are specified within the stratiform model. In fact, they should be related to the host-code defined horizontal wind flow, since the stratiform clouds are assumed to occupy an area comparable to that of the host code cell in which the RSM is operating. The absence of such data during development of the stratiform operator cloud precluded implementation of this refinement.

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APPENDIX A

REFERENCES FOR SOLUBILITY AND DISSOCIATION PARAMETERS

Following is a list of references used in compiling the solubility and dissociation parameters used in the RSM. References were limited to works which presented actual data or treatments of previously published data. Modeling related articles are occasionally listed when they were helpful in locating original sources.

An asterisk (*) indicates that the data contained in the indicated article was referenced heavily in the preceding citation.

The authors of this report are indebted to E.G. Chapman of Pacific Northwest Laboratory for preparation of this list.

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* Wagman, D. D., W. H. Evans, V. B. Parker, I. Halow, S. M. Bailey and R. H. Schum. 1968. "Selected Values of Chemical Thermodynamic Properties. Tables for the First Thirty-four Elements in the Standard Order of Arrangement." US NBS Technical Note 270-3, National Bureau of Standards, U.S. Department of Commerce, Washington, D.C.

NH_3:

Hales, J. M., and D. R. Drewes. 1979. "Solubility of Ammonia in Water at Low Concentrations." Atmos. Environ. 13:1133-1147.

Ayers, G. P., R. W. Gillett and E. R. Caeser. 1985. "Solubility of Ammonia in Water in the Presence of Atmospheric CO_2." Tellus. 37(b):35-40.

CO_2:

Harned, H. S. and R. Davis. 1943. "The Ionization Constant of Carbonic Acid and the Solubility of Carbon Dioxide in Water and Aqueous Salt Solutions from 0 to 500," Am. Chem. Soc. J. 65:2030-2037.

Stumm, W. W., and J. J. Morgan. 1970. Aquatic Chemistry. John Wiley & Sons, New York.

O_3:

Wagman, D. D., W. H. Evans, V. B. Parker, I. Halow, S. M. Bailey, and R. H. Schum. 1968. "Selected Values of Chemical Thermodynamic Properties. Tables for the First Thirty-four Elements in the Standard Order of Arrangement." US NBS Technical Note 270-3, National Bureau of Standards, U.S. Department of Commerce, Washington, D.C.

Perry, J. H., R. H. Perry, C. H. Chilton and S. D. Kirkpatrick, eds. 1980. Chemical Engineers Handbook. MacGraw-Hill, New York.

Chameides, W. L. 1984. "The Photochemistry of a Remote Marine Stratiform Cloud." J. of Geophysical Res. 89:4739-4755.

H_2O_2:

Martin, L. R., and D. E. Damschen. 1981. "Aqueous Oxidation of SO_2 by H_2O_2 at Low pH." Atmos. Environ. 15:1615-1621.

* Scatchard, G., G. M. Kavanagh and L. B. Ticknor. 1952. "Vapor-Liquid Equilibrium. VIII. Hydrogen Peroxide-Water Mixtures," J. of the Am. Chem. Soc. 74:3715-3720.

H_2S:

Stephen, H., and T. Stephen, eds. 1963. Solubilities of Inorganic and Organic Compounds, Vol. 1 of Binary Systems. Pergamon Press, New York.

* Wright, R. H., and O. Maass. 1932. Canadian J. of Res. 6:94.

HCl

Weast, R. C., ed. 1984. CRC Handbook of Chemistry and Physics. CRC Press, Inc., Boca Raton, Florida.

CH_2O

Wagman, D. D., W. H. Evans, V. B. Parker, I. Halow, S. M. Bailey and R. H. Schum. 1968. "Selected Values of Chemical Thermodynamic Properties. Tables for the First Thirty-four Elements in the Standard Order of Arrangement," US NBS Technical Note 270-3, National Bureau of Standards, U.S. Department of Commerce, Washington, D.C.

Chameides, W. L., and D. D. Davis. 1983. "Aqueous-phase Source of Formic Acid in Clouds." Nature. 304:427-429.

Kw (Equilibrium Constant for Water)

Weast, R. C., ed. 1984. CRC Handbook of Chemistry and Physics. CRC Press, Inc., Boca Raton, Florida.

Activity Coefficient Parametrizations (Based on ionic strength of solution)

Stumm, W., and J. J. Morgan. 1970. Aquatic Chemistry. John Wiley & Sons, New York.

APPENDIX B

GLOSSARY OF TERMS USED IN SUBROUTINES DESCRIPTION

The following annotated list is based on variables referenced in Appendix C, "Subroutine Description." It does not include many of the internal variables of the scavenging module.

Easter and Hales (page 17, 1984) introduce the concepts of computed variables, constrained variables, "species index" and "species location variable". This distinction has been maintained in the scavenging module. Chemical species are identified by their standard chemical notation. However, references will be found in this manual which makes use of the following postscript notation used to define the media in which such species are carried: for species "xxx":

Kxxx|g = gasborne form of this species
Kxxx|r = rainborne form of this species
Kxxx|s = snowborne form of this species
Kxxx|a1 = aerosol form of species available for cloud nucleation (a1)
Kxxx|a2 = aerosol form of species not available for scavenging (a2)
Kxxx|c = cloudborne form of this species
Kxxx|gc = g+c
Kxxx|alc = a1+c
Kxxx|galc = g+a1+c

With this notation, the interpretation of the following species location variables in Table B-1 should be clear.

The index variable K refers to height and L to species. Many arrays in the PLUVIUS II code were originally dimensioned in (I,J,K) or (I,J,K,L), where I and J are indices for two horizontal directions, as the code was intended to operate on a 3-D grid. Within the RSM, the I index is not used (I = 1 for these variables) and the J index refers to different cells within the RSM, not to a horizontal coordinate. Thus, these PLUVIUS II arrays are shown with dimension (1,J,K) and (1,J,K,L).

An asterisk (*) indicates reference to the introductory notes of this glossary.

TABLE B-1. LIST OF CHEMICAL SPECIES RELATED VARIABLES IN THE RSM.

Species	Species Location Variable Name	Chemical Species	Form of Species
Computed Variables			
1.	KSO2GC	SO_2	gas + cloud
2.	KSO2R	SO_2	rain
3.	KSO2S	SO_2	snow
4.	KH2O2GC	HOOH	gas + cloud
5.	KH2O2R	HOOH	rain
6.	KH2O2S	HOOH	snow
7.	KSO4A1C	SO_4	a1 aerosols + cloud
8.	KSO4A2	SO_4	a2 aerosols
9.	KSO4R	SO_4	rain
10.	KSO4S	SO_4	snow
11.	KCATNA1C	lumped cation	a1 aerosols + cloud
12.	KCATNA2	lumped cation	a2 aerosols
13.	KCATNR	lumped cation	rain
14.	KCATNS	lumped cation	snow
15.	KNO3GA1C	NO_3	a1 aerosols + cloud
16.	KNO3A2	NO_3	a2 aerosols
17.	KNO3R	NO_3	rain
18.	KNO3S	NO_3	snow
19.	KNH4GA1C	NH_4	a1 aerosols + cloud
20.	KNH4A2	NH_4	a2 aerosols
21.	KNH4R	NH_4	rain
22.	KNH4S	NH_4	snow
23.	KO3G	O_3	gas
Constrained Variables			
24.	KTEMP	temperature	
25.	KVAPCL	H_2O	water vapor + cloud
26.	KRAIN	H_2O	rain
27.	KSNOW	H_2O	snow
28.	KCLOUD	H_2O	cloud
29.	KCLDICE	H_2O	cloud ice (not used)
30.	KHIONC	H^+ ion	cloud
31.	KHIONR	H^+ ion	cloud
32.	KSO2G	SO_2	gas
33.	KSO2C	SO_2	cloud
34.	KSO4A1	SO_4	a1 aerosols
35.	KSO4C	SO_4	cloud
36.	KCATNA1	lumped cation	a1 aerosols
37.	KCATNC	lumped cation	cloud
38.	KNO3G	NO_3	gas
39.	KNO3A1	NO_3	a1 aerosols
40.	KNO3C	NO_3	cloud
41.	KNH4G	NH_4	gas
42.	KNH4A1	NH_4	a1 aerosols
43.	KNH4C	NH_4	cloud
44.	KH2O2G	HOOH	gas
45.	KH2O2C	HOOH	cloud

Variable	Description
ALPHxxx	The α in Eqs. 34-36, where "xxx" refers to species. See description of Subroutine RAIN_INIT for definition of "xxx" (dimensionless).
AREA(J)	Area associated with each cell of the scavenging module (cm^2)
CAIR(1,J,K)	Air concentration ($moles/cm^3$).
CNN(L)	Holding array for species concentrations ($moles/cm^3$) at a "current" cell and height.
CONC(K,KKxxxC)	Holding array for species concentration in top down integration of RAIN_INIT.
CS(K)	Air concentration ($moles/cm^3$) in a current cell.
DELTA_xxx(J)	Mass of species "xxx" in column j that has been removed by wet removal. Species "xxx" defined in Subroutine DELTA_MASS notation in "Subroutine Descriptions" ($moles/cm^2$).
DSUNIF	Vertical grid interval. Defined in Subroutine INPUTMET (cm).
DT	Time interval of integration step in Subroutine CORE (seconds).
DZ	Vertical grid interval (cm) (= DSUNIF).
F(JDET,JENT,K)	$F_{jm}(Z)$ in Eq. 8. JDET is cell from which mass is being detrained, JENT is cell to which mass is being entrained (moles/cm - sec).
FALSPD	Fall speed of precipitation particles (rain or snow depending on temperature) in Function SCAVCOEF (cm/s).
FNUCCATN	Fraction of cation aerosol available for nucleation scavenging (dimensionless).
FNUCNH4	Fraction of ammonium aerosol available for nucleation scavenging (dimensionless).

FNUCNO3	Fraction of nitrate aerosol available for nucleation scavenging (dimensionless).
FNUCSO4	Fraction of sulfate aerosol available for nucleation scavenging (dimensionless).
IHOUR_RADM	Time index for data being read from host code meteorological data file (see "Input Data").
IMAXMM4	Maximum east - west index of host code code.
IRADM	East - west index of RADM.
I_RADM	East - west index of scavenging module = IRADM.
JDET	See F(JENT,JDET, K).
JENT	See F(JENT,JDET,K).
JMAXMM4	Maximum north - south index of host code code.
JRADM	North - south index of RADM.
J_GRID,	North - south index of scavenging module.
KCALL	Counter for the number of times a given subroutine has been called.
KDIAG	Internal flag for diagnostic studies. Not intended for user modification.
KDIAG_OLD	User defined flag for diagnostic studies. When >0, values of key variables printed; <0, no such printing occurs. Read from file LUNIN.
KFIRSTLTØ	Vertical index associated with the first layer having temperature less than 0°C. Used in Subroutine INIT STRATI.
KNRSCAV	User defined flag. Read from file LUNIN. When > 0, nonreactive scavenging processes enabled; < 0, nonreactive scavenging processes switched off (no mass transfer by cloud microphysics).

KRSCAV	User defined flag. Defined in file LUNIN. When > 0, reactive scavenging processes enabled; < 0, reactive scavenging processes switched off (no aqueous phase chemistry or mass transfer).
KSTORM	Index associated with host code layer at which stratiform cloud top is located.
KTOP	Upper index of DO loop over height.
KTRANS	User defined flag. Defined in file LUNIN. When > 0, vertical transport is enabled; < 0, vertical transport is switched off.
LTOT	Number of computed species in RSM.
LTOT2	Number of constrained species in RSM.
LUNIN	Logical unit number of input data file read by Subroutine INPUT1. Last line of this file contains variables KDIAG OLD, KTRANS, KRSCAV and KNRSCAV.
MULT	Flag for enabling ice multiplication mechanism (see Scott 1986a).[1]
NAME(M,L)	Holds alphanumeric mnemonic species names used in printing out values related to species L. Up to 10 letters allowed in these mnemonic codes.
OLDTOTAL	In MASS_SUM, the column integral of mass (moles/cm^2) associated with a species at the start of the simulation.
PCB	Pressure at cloud base (dynes/cm^2).
PGROUND	Pressure at the ground (dynes/cm^2). Defined by host code.
PHI(K)	ϑ in Eq. 25
PRATE_STRATI(K)	Holding array for precipitation rate from stratiform cloud (mm/h).

[1]Scott, B. C. 1986a. "User's Manual for the Cloud and Scavenging Module." (In preparation.)

PRESS(K)	Air pressure in current column (dynes/cm^2).
PTOT(1,J,K)	Air pressure (dynes/cm^2).
P_OUTSIDE (K)	RADM based pressure interpolated to RSM grid (dynes/cm^2).
P_RADM(K)	Pressure on RADM vertical grid (dynes/cm^2).
QV_OUTSIDE (K)	RADM based mixing ratio interpolated to RSM grid (g/g).
QV_RADM(K)	Mixing ratio on RADM vertical grid (grams of vapor/grams of air).
R(1,J,K,L)	Molar mixing ratio (mole of species/(moles/air).
R(1,J,K,KTEMP)	Air temperature (K).
RATE(J,K,IRATE)	Cloud microphysical mass transfer rate (s^{-1}). IRATE is defined from the following list: IRATE = KAUTO = 1 is autoconversion rate. IRATE = KMELT = 2 is melting rate. IRATE = KEVAP = 3 is evaporation rate IRATE = KFREEZ = 4 is freezing rate IRATE = KDEP = 5 is deposition rate IRATE = KRIM = 6 is riming rate IRATE = KSUB = 7 is sublimation rate IRATE = KACCRET= 8 is accretion rate.
RC_RADM	Host defined precipitation associated with convection over previous hour of simulation (cm/h).
RH	Relative humidity (dimensionless).
RHG	Relative humidity at ground (dimensionless).
RT_RADM	Host defined total precipitaion over previous hour of simulation (cm/h).
SCAV	Either a riming rate or accretion rate, depending on temperature (s^{-1}).
SUMRAIN	Column integral of rain borne species (moles/cm^2) (see RAIN_INIT).

SUMTOT	Sum of all column integrals of species mass in scavenging module (moles/cm^2).
SUMxxx	Column integral of species "xxx" (moles/cm^2) (see RAIN INIT).
T	Time into RSM simulation (seconds).
TØ	Surface temperature for CLOUD_STRATI (C) (see Scott 1986a).[1]
T2	Temperature of parcel lifted moist adiabatically (K).
TCB	Cloud base temperature (K).
TCONVT	Temperature of precipitating convective cloud top (K).
TDAB	Temperature of parcel lifted dry adiabatically (K).
TEMP(K)	Column array of temperature (K).
TEMPERC	Centigrade equivalent of a (K) temperature.
TEMP_STRATI(K)	Holding array for temperature from stratiform cloud (K).
TG	Ground temperature for stratiform cloud calculations (C) (see Scott 1986a).[1]
TGROUND	Ground temperature from host code (K).
TOTAL	In MASS_SUM, the column integral of mass (moles/cm^2) associated with a species at the end of the simulation.
T_OUTSIDE (K)	RADM based temperature interpolated to RSM grid (K).
TPRIME	Temperature of a lifted parcel (K).
TT	Stratiform cloud top temperature (C) (see Scott, 1986a).[1]
T_RADM(K)	Temperature on RADM vertical grid (K).
U_RADM(K)	Host-code-defined west-to-east winds on RADM grid (cm/s).

[1]Scott, B. C. 1986a. "User's Manual for the Cloud and Scavenging Module." (In preparation.)

VERTCL(I,J,K,2)	Fall speed of rainborne species (cm/s).
VERTCL(I,J,K,3)	Fall speed of snowborne species (cm/s).
V_RADM(K)	Host-code-defined south-to-north winds on RADM grid (cm/s).
WC	Area weighted average of the two convective updrafts (cm/s).
WE	Updraft associated with non-convective region (cm/s).
WET_xxx(J)	Mass of species "xxx" removed by wet removal (moles/cm^2). See Subroutine DELTA_MASS.
WINDS(I,J,K)	Vertical wind speed of air in scavenging module (cm/s).
WMM4	Host-code-defined updraft, interpolated to a height coordinate of the scavenging module (cm/s).
W_OUTSIDE (K)	RADM based updraft interpolated to RSM grid (cm/s).
W_RADM(K)	Host-code-defined vertical winds on RADM grid (cm/s).
X(3,K)	Vertical coordinate of RSM grids (cm).
XJO	Surface precipitation rate in stratiform cloud model (mm/h) (see Scott 1986a).[1]
XNO	Intercept of Marshall-Palmer Distribution (m^{-4}) (see Scott 1986a).[1]
Z(K)	Column array of heights within the scavenging module (cm).
ZCB	Height of cloud base (cm).
ZLZ(K)	Height array within stratiform cloud (m).
Z_METERS	Local variable for using height in units of (m).

[1]Scott, B. C. 1986a. "User's Manual for the Cloud and Scavenging Module." (In preparation.)

Z_RADM(K)	Column array of heights associated with the host code sigma layers (cm above ground level).
ZSTORM	Local variable for height of storm (cm.).
ZTOP(J)	Cloud top height (cm).

APPENDIX C

SUBROUTINE DESCRIPTIONS

The glossary in Appendix B contains definitions of variables given in the following description of subroutines. Table 3 shows the calling sequence of these routines. The units associated with these variables are as indicated in Appendix B unless noted otherwise.

The following format has been selected for general documentation of subroutines:

Subroutine NAME (= "explanation of any mnemonic methods associated with the name")

a. Function: a list of functions this subroutine is intended to provide to the scavenging module. Reference may be made to other parts of this user's guide in defining such functions (i.e., evaluation of a certain term in an equation presented elsewhere in the user's guide)

b. Design Constraints: a list of constraints or known problems associated with this subroutine. Optional.

c. User Interaction: a list of ways by which the user of the scavenging module is expected to modify this subroutine. Optional. This will usually refer only to implementing the option of printing out key variables in the subroutine. The units of variables referred to are those given in the glossary, unless noted otherwise.

d. Key Algorithms: a list of the key algorithms in this subroutine. This list may reference variables not contained in the glossary, but such variables will be defined herein. Reference may be made to other parts of this user's guide in defining such algorithms. The units of variables referred to are those given in the glossary, unless noted otherwise.

****

PROGRAM RADM:

A short code consisting of a DO loop to cycle through several soundings provided by NCAR. This short routine is intended to emulate the programming environment in which the RSM will be called.

****

SUBROUTINE RSM (= RADM Scavenging Module)

Function:

a. The governing subroutine of the RADM Scavenging Module.

b. No calculations are done within this module.

c. Upon the first call from RADM, Subroutines BLOCKDATA and INPUT1 are called.

d. Following call to INPUTMET, if no precipitation or fair weather cumulus fields are defined, then control is returned to RADM. The basis for this test is the value of AREA(J), which must be greater than 0.001 to avoid return of control to RADM.

e. DSUNIF defined as MAX (ZTOP(1), ZTOP(2), ZTOP(4))/19).

Design constraints:

a. IRADM ≤ IMAXMM4, JRADM ≤ JMAXMM4 (see glossary).

****

SUBROUTINE BLOCKDATA (= Block Data statements)

Function:

a. Data statements define variables necessary for all applications of the RSM. These variables are intended for internal use; they should not be adjusted by the user.

Design Constraints:

a. It is up to the user to be sure that the values defined in this module are not redefined in subsequent parts of the code.

```
**************************************************************************
SUBROUTINE INPUT1 (= Input routine 1)

Function:

 a. To define variables necessary for all applications of the RSM.
    These variables were routinely modified during development of the
    RSM.

Design constraints:

 a. It is the responsibility of the user not to redefine these
    variables in subsequent parts of the code.

 b. It is the responsibility of the user to define logical file LUNIN
    for access by this module.

**************************************************************************
Subroutine GRDXYZ (='Grid:  x, y & z')

Function:

 a. Defines horizontal and vertical grid spacing in RSM Design
    Limitations:
      1. climatological values used for DYUNIF
      2. DXUNIF is not used
      3. DSUNIF defined in INPUTMET

User Interaction:

 a. If KDIAG > 0, then the following variables printed out as a summary
    of a result of the calculations in GRDXYZ
      1. DSUNIF, X(3,K)

**************************************************************************
SUBROUTINE INPUTMET (= Input:  Meteorological Data)

Function:

 a. To zero out arrays of mixing ratio, cloud top height, fractional
    cloud area and fluxes, prior to RSM simulation.

 b. To call subroutines related to defining the meteorological initial
    conditions.
```

Design constraints:

a. Not intended for modification by the user.

User Interaction:

a. KDIAG >0 produces printout of following values:[1]
   1. I_RADM, J_RADM
   2. ZTOP(1)
   3. TGROUND - 273.15 (C)
   4. ZCB
   5. XJO,
   6. PGROUND/1000 (mb)
   7. RHG

****

Subroutine INPUT_MM4 (= Input: MM4 data)

Function:

a. Upon the first call from INPUTMET, calls READMET.

b. Transfers host code defined values of rainfall rate, surface temperature and vertical profiles of temperature, moisture and winds, into RSM defined variables. Unit conversions also done.

c. Estimates geometrical height of host code sigma coordinates (see Anthes 1985).

d. KDIAG > results in Subroutine TPLOT being called.

Design constraints:

a. Units from host code must be defined as per correspondence from Walcek (1986b).

Key Algorithms:

a. Uses mean temperature of host code layers in hydrostatic equation to estimate geometrical height of host code sigma levels.

---

[1]Units of printed values are as indicated in glossary unless noted otherwise.

User Interaction:

a. KDIAG > 0 produces printout of following values:[1]
   1. I_RADM, J_RADM, IHOUR_RADM
   2. TGROUND - 273.15 (C)
   3. PGROUND/1000 (mb)
   4. RC_RADM*10 (mm)
   5. RT_RADM*10 (mm)
   6. Z_RADM*1.E-5 (cm)
   7. P_RADM/1000 (mb)
   8. T_RADM-273.15 (C)
   9. QV_RADM*1000. (g/kg)
   10. U_RADM/100, V_RADM/100 (m/s)
   11. W_RADM

****

Subroutine READMET (= Read Meteorology data)

Function:

a. To read files provided by host code.
b. To define updraft in host grid I_RADM, J_RADM.

Design Constraints:

a. Input data is expected to be defined as those in section 3.5 of this report.

User Interaction:

a. See section 3.5.

Key algorithms:

a. Mass continuity equation in sigma coordinates integrated to calculate updrafts. See documentation by Walcek (1986).

[1]Units of printed values are as indicated in glossary unless noted otherwise.

****

Subroutine TPLOT (= Temperature Plot)

Function:

a. To determine the meteorological stability class of each layer of the host code defined profile of temperature lapse rate.

b. Parcel stability values at each layer printed out. (See page 100 of Hess,' 1959.)

Design Constraints:

a. Units of variables from host code must be defined as per Walcek (1986).

Key algorithms:

a. Host code defined lapse (dT/dP) compared with moist lapse rate and dry lapse rate.

User Interaction:

a. Called only when KDIAG >0.

****

Subroutine STABCLASS (= Stabillity Class)

Function:

a. To sets flag for printing meteorological stability class.

User Interaction:

a. Called from TPLOT when KDIAG >0.

****

Subroutine CLOUD_BASE (='Cloud Base')

Function:

a. Calculates the common cloud base for all four RSM cells. This height is defined as the lifting condensation level from temperature and moisture values defined at the lowest layer of the host code.

b. Temperature, pressure and an estimate of geometrical height (using a hypsometric relation) are also calculated.

Design Constraints:

a. Mixing ratio at lowest layer of host code is required to be no greater than its saturation value.

Key Algorithm(s):

a. A fourth order Runge-Kutte integrator (Carnahan, Luther and Wilkes 1969) is used to calculate the dry adiabatic temperature from a parcel lifted from the lowest layer of the host code:

$$T_{DAB} = T_0 + \int_p dp \left(\frac{dT}{dp}|dry\right)$$

$$= T_0 + \left(-\frac{1}{cp}\right) \int_p \frac{dp}{\rho}$$

The associated saturation mixing ratio is calculated using Function ESAT and the ideal gas law. If this value is greater than the mixing ratio at the lowest layer of the host code, than interpolation over ln[(p(k)/p(k-1)] is done to find the pressure height at which the lifted mixing ratio equals the mixing ratio at the lowest layer.

b. A similar interpolation is done for temperature and geometrical height.

User Interaction:

a. If KDIAG > 0, then the following values are printed:
   1. host code height index for cloud base
   2. ZCB/1.E5 (km)
   3. PCB/1000 (mb)
   4. TCB-273.15 (C)

****

Function ESAT (= Es, standard meteorological notation for vapor pressure)

Function:

a. To calculate saturation vapor pressure from specified temperature.

b. Documentation in Easter and Hales (1984).

****

Function TEMP_LIFTED_DRY (= Temperature of Parcel, lifted dry adiabatically)

Function:

a. To calculate temperature of a parcel lifted dry adiabatically.

Key Algorithms:

a. Fourth-order Runge-Kutte integrator used to lift parcel over pressure interval defined by calling argument.

b. Change in temperature with pressure given by Function DTDPDRY.

****

Function DTDPDRY (= dT/dP|dry)

Function:

a. To define dry adiabatic lapse rate [K/(dynes/cm^3)]

Key Algorithms:

a. Hydrostatic equation and equation of state used to convert from dT/dz = g/cp, to dT/dP, where T,z,g and c_p represent temperature, height, acceleration of gravity and specific heat at constant pressure. Cgs units assumed.

****

Subroutine CONVCLD_TOP (='Convective Cloud Top')

Function:

a. Calculates convective cloud top height for RSM grid cells 2 and 3.

User Interaction:

a. Called only if user defined convective precipitation rate is non-zero.

b. If KDIAG > 0, then the following variables are printed: they are intended to be diagnostic of problems which may enter into the final calculation of cloud top:
   1. k, = vertical grid index.
   2. Z_RADM(k) (km)
   3. P_RADM(k) (mb)

4. T_RADM(k)-273.15 (C)
5. T2-273.15 (C)

c. If KDIAG > 0, then the following variables are printed; they are intended to summarize the results of the calculations in Subroutine CONVCLD_TOP:
   1. ktop, = vertical grid index of cloud top
   2. ZTOP(2) (km)
   3. P_RADM(KTOP)/1000 (mb)
   4. TCONVT-273.15 (C)

Design Limitations:

a. If the host-code uses soundings from a mesoscale model which removes instability during the sub-one hour integration steps, then no level of neutral buoyancy can be defined.

Key Algorithms:

a. LNB is calculated by comparing temperature of host-code against the quantity

$$T'_0 + \int dp \left(\frac{dT}{dp}\Big|_{moist}\right)$$

at each layer of the host-code sounding. The LNB is approximated by the highest level at which T' > the host-code temperature.

b. If T' always < the host-code temperature, the convective cloud top is defined by the host-code values at layer 6 (approximately 6 km).

****

Subroutine CLOUD_CONV (='Cloud: Convective')

Function:

a. To define the scavenging environments in RSM cells 2 and 3.

b. Documentation to be provided by Scott (1986b).[1]

---

[1]Scott, R. D. 1986b. "User's Manual for the Convective Storm Component of the RSM." (In preparation.)

****

Subroutine INIT_CONV (='Initialization: Convective storm')

Function:

a. To interface results from CLOUD_CONV with RSM.

****

Subroutine CLOUD_TOP (='Cloud Top: stratiform')

Function:

a. Calculates average updraft at each layer for both the convective updraft and downdraft operator clouds.

b. Uses the results of a) and b) to evaluate $w_{nonconv}$ (Eq. 23 in "Definition of the Updraft in the Stratiform Region").

c. Defines the stratiform cloud top height and updraft (Eq. 19 in "Definition of the Updraft in the Stratiform Region").

Key algorithms:

a. See "Definition of the Updraft in the Stratiform Region."

User Interaction:

a. If KDIAG > 0 then the following variables are printed out as an aide in identifying problems that may arise in calculations in CLOUD_TOP:[1]
   1. kstorm
   2. zstorm
   3. we
   4. wmm4
   5. wc
   6. RH
   7. TPRIME - 273.15 (C)

b. If KDIAG > 0 then the following variables are printed out to summarize the results of the calculatations in CLOUD_OP:
   1. Vertical index number
   2. zstorm (cm)
   3. winds(,1,k)

---

[1]Units of printed values are as indicated in glossary unless noted otherwise.

****

Function TEMP_LIFTED (='Temperature Lifted moist adiabatically')

Function:

a. To calculate temperature of parcel lifted moist adiabatically over pressure interval specified in calling argument.

Key Algorithms:

a. Fourth-order Runge-Kutte integration (Carnahan, Luther and Wilkes, 1969) of Eq. 2.101 in Fleagle and Businger (1980).

****

Subroutine MM4_TO_RSM (='MM4 to RSM interpolation')

Function:

a. Interpolates MM4 variables at specified σ levels to vertical grid of RSM.

b. Interpolated variables include: pressure, temperature, moisture, and winds.

User Interaction:

a. If KDIAG > 0, then the following variables are printed to check on consistency between height and pressure values of host code and RSM:[1]

1. X(3,20) (km)
2. ZCB (km)
3. K (RSM height index),
4. X(3,k) (km)
5. P_OUTSIDE (K) /1000 (mb)
6. T_OUTSIDE (K) -273.15 (C)
7. CAIR (I,I,K)
8. W_OUTSIDE (K)
9. QV_OUTSIDE (K)

[1]Units of printed values are as indicated in glossary unless noted otherwise.

****

Subroutine CLOUD_STRATI (='Cloud: stratiform')

Function:

a. Governs calling of subroutines needed to define stratiform scavenging environment.

b. Documentation contained in Scott (1986a).[1] RSM Subroutine CLOUD STRATI is based on Scott's Subroutine STMAIN.

c. CLOUD_STRATI differs from STMAIN in the following characteristics:

   1. The height and pressure are defined to be those of the RSM system (X(3,K) and PTOT(1,1,K).

   2. The calculations in CLOUD_STRATI are done for a defined surface temperature (rather then a series of such temperatures), a defined storm height (rather then a series of such heights) and a defined surface rainrate (rather then a series of such rates).

d. The user is referred to the section 6 of this report, item 6, for characteristics of this subroutine which will be modified in subsequent versions of the RSM.

User Interaction:

a. If KDIAG > 0, the following variables are printed as an aide to identifying problems associated with this subroutine:[2]
   1. TG, TT, XNO, MULT, NOPRE
   2. K,*
   3. ZLZ(K)
   4. PRESS(K)/1000 (mb)
   5. TEMP(K),
   6. TEMP_STRATI(K)

---

[1]Scott, B. C. 1986a. "User's Manual for the Cloud and Scavenging Module." (In preparation.)

[2]Units of printed values are as indicated in glossary unless noted otherwise.

****

Subroutine SIGMA_BCS (='Sigma, B. C. Scott')

Function:

a. To define the stratiform temperature and air density profile (cell 1).

b. Full documentation in Scott (1986a).[1] SIGMA_BCS corresponds to Subroutine SIGMA in Scott. The height and pressure levels of the RSM are employed, rather than the values defined by Scott.

User Interaction:

a. If KDIAG > 0, then the following variables are printed out. They are intended as use for diagnostic analysis of problems.[2]
   1. K, height index in stratiform cell
   2. Z(K) (cm)
   3. PRESS(K)/1000 (mb)
   4. TEMP(K)

****

Subroutine INIT_STRATI (='Initialization: stratiform')

Function:

a. Transfers variables defined by CLOUD_STRATI to variables used in CORE and other RSM subroutines.

Key Algorithms:

a. Height index of the first layer from ground which has a temperature less than freezing (KFIRSTLTO = "K first layer less than zero") is located (this index used in subsequent part of code to determine if scavenging should be accretion or riming, and if fall speed should be that of rain or snow).

b. Air density in stratiform region defined to be consistent with temperature and pressure defined in SIGMA_BCS.

---

[1] Scott, B. C. 1986a. "User's Manual for the Cloud and Scavenging Module." (In preparation.)

[2] Units of printed values are as indicated in glossary unless noted otherwise.

c. Melting and freezing rate set to minimum value (see section 6 in this report).

User Interaction:

a. For KDIAG > 0, the following variables are printed. They are intended for diagnostic use in the RSM.[1]

1. K, vertical grid index for stratiform region.
2. TEMPERC
3. z_meters
4. CAIR(1,J_GRID,K)
5. PTOT(1,J_GRID,K)/1000 (mb)
6. RATE(1,K,IRATE) (array of microphysical rates). See listing of Subroutine BLOCKDATA for mapping of IRATE to specific microphysical process.
7. FALSPD/100
8. PRATE_STRATI(K)
9. R(1,J_GRID,K,KCLOUD)*18.E6*CAIR(1,J_GRID,K) (m^3)
10. WINDS(1,J_GRID,K)

****

For stratiform cloud thickness less than 1.5 km:
Subroutine CUVENT (='Cumulus Venting')

Function:

a. To define scavenging environment in RSM cells 1 and 4 when host code updraft and CLOUD_STRATI microphysics define a non-convective precipitation rate less than 0.01 mm/h.

---

[1]Units of printed values are as indicated in glossary unless noted otherwise.

b. Not yet implemented in the RSM. See documentation by Vukovich (1986).[1]

****

Subroutine GRDSET (='Grid Setup')

Function:

a. Computes grid expansion factors and common grid terms for subsequent use in numerical approximations. Interrogated only once during program execution.

b. Documentation available from R. C. Easter (PNL).

Key Algorithms:

a. To be described by R. C. Easter. Differs from original work of Easter by defining only those terms necessary for the vertical array.

****

Subroutine INIT (='Initialization of chemistry')

Function:

a. Governs calling of RSM subroutines associated with initialization of chemistry (Subroutines INPUT_RADM and RAIN_INIT).

b. Defines internal variables necessary to use PLUVIUS MOD. 5.0 routines.

****

Subroutine INPUT_RADM (='Input from RADM')

Function:

a. A dummy subroutine designed to emulate the initialization of clear air chemistry values defined by the host code.

b. This initialization is performed uniformly over all the RSM grids at all vertical layers.

---

[1]Vukovich, F. 1986. "User's Guide to CUVENT." (In preparation.)

Design Limitations:

a. Mixing layer height arbitrarily defined; see section 6.

Key Algorithms:

a. Data statements at the beginning of the program define representative (ppb) values of planetary boundary layer and upper air pollutants associated with: KSO2GC, KSO4A1C, KSO4A2, KCATNA1C, KCATNA2, KNO3GA1C, KNO3A2, KNH4GA1C, KNH4A2, KH2O2GC and KO3G.

b. Fraction of aerosols (i.e., FNUCSO4, FNUCCATN, FNUCNO3, AND FNUCNH4) available for cloud nucleation used to define A1C species (see glossary).

c. Clear air values of NO_3 and NH_4 (KNO3G and KNH4G) defined.

User Interaction:

a. If KDIAG > 0, then the following values are printed out. They are intended as an aide in diagnosing problems that may be associated with the initial conditions in the RSM:[1]

1. R(1,J,K,KSO2GC)
2. R(1,J,K,KSO4A1C)
3. R(1,J,K,KSO4A1C)
4. R(1,J,K,KSO3A2)
5. R(1,J,K,KCATNA1C)
6. R(1,J,K,KCATNA2)
7. R(1,J,K,KNO3GA1C)
8. R(1,J,K,KNO3A2)
9. R(1,J,K,KNH4GA1C)
10. R(1,J,K,KNH4A2)
11. R(1,J,K,KH2O2GC)
12. R(1,J,K,KO3G)

****

Subroutine RAIN_INIT (='Rain Initialization for chemistry')

Function:

a. To initialize aqueous phase chemistry.

---

[1]Units of printed values are as indicated in glossary unless noted otherwise.

b. Theoretical basis for this initialilzation is presented in section 2.6 of this report.

Design Limitations:

a. Initialization procedure is identical for all regions of RSM.

b. Only those regions with AREA(J) greater than the arbitrarily small number of 0.001 undergo this initialization.

Key Algorithms:

a. For each region of the RSM, CALLGEN is called to initialize the cloud borne concentration of species.

b. Equation 33 is the key algorithm in this subroutine.

c. The variables ALPHxxx define the α's in Eq. 34, where xxx represents the associated species. In a loop over height, the concentrations (moles/cm^3) are multiplied by the appropriate ALPHxxx to complete the third phase of the aqueous phase chemistry initialization. Within this same section of code, snowborne species are defined (the algorithm has depended on temperture only through Functon SCAV up to this point).

d. The final stage of the algorithm is redefinition of the computed species so they equal the sum of their partitioned counterparts. CALLGEN is called at the very end to readjust the equilibria concentrations of the cloud-borne components.

User Interaction:

a. If KDIAG > 0, then the concentration units in RAIN_INIT are used to print the following values:[1]

   1. K, vertical height index

   2. CONC(K,KKxxxC), (moles/cm^3) where xxx is: H_2O_2, SO_4, CATN, NO_3, NH_4, SO_2

   3. SUMxxx (moles/cm^2)

[1]Units of printed values are as indicated in glossary unless noted otherwise.

4. SUMRAIN

5. SUMTOT

6. ALPHxxx (dimensionless)

b. If KDIAG >0, then Subroutine RIDIAG (='Rain Initialization Diagnostics') is called. Mixing ratio units from RAIN_INIT are used to print values analogous to those listed in a). In addition, the following values are printed.[1]
   1. Z(K) (km)
   2. R(1,J,K,KTEMP) - 273.15 (C)
   3. DZ (km)
   4. VERTCL(1,J,K,KAT)
   5. SCAV
   6. CAIR(1,J,K)
   7. RATE(J,K,KACCRET)
   8. RATE(J,K,KRIM)

****

Function SCAVCOEF (='Scavenging Coefficient')

Function:

a. To define the scavenging rate S' in Eq. 31. S = the riming rate for temperatures below freezing and the accretion rate for temperature above freezing.

Key Algorithms:

a. For temperatures greater than freezing, the fall speed of rain at height grid K is used, and the accretion rate is used for the scavenging rate.

b. For temperatures less than freezing, the fall speed of snow at height grid K is used, and the riming rate is used for the scavenging rate.

[1]Units of printed values are as indicated in glossary unless noted otherwise.

****

Subroutine CALLGEN (='Call to GEN')

Function:

a. Prepares arrays for call to Subroutine GEN by

   1. Loading concentration (moles/cm^3) equivalent of mixing ratio values into array CNN.

   2. Loading PTOT and CAIR arrays into PLUVIUS column equivalent arrays of PRESS and CS.

b. Calling Subroutine GEN.

c. Unloading CNN, PTOT and CAIR to R, PRESS and CS after call to GEN.

****

Subroutine GEN (='Generation and decay')

Function:

a. To compute the generation and decay rates for the computed species.

b. To set constrained species (see Subroutine RAIN_INIT).

c. To call subroutines which define the cloud microphysical transfer rates (MICRO) and equilibrium cloud-air concentrations (AQEQUIL).

d. To call subroutines which compute rates for nucleation scavenging, mass transfer between gas and rainborne species and chemical reaction of aqueous species.

****

Subroutine MICRO (='Microphysics')

Function:

a. Loads the RSM column rates of autoconversion, melting, evaporation, freezing, deposition, riming, sublimation and accretion into variables used in generation and decay terms of following species:
   SO_2|gc, SO_2|r, SO_2|S,
   HOOH|gc, HOOH|r, HOOH|s
   SO_4|a1c, SO_4|a2, SO_4|r, SO_4|s,
   CATN|a1c, CATN|a2, CATN|r, CATN|s
   NO_3|ga1c, NO_3|a2, NO_3|r, NO_3|s,
   NH_4|ga1c, NH_4|a2, NH_4|r, NH_4|s.

****

Subroutine AQUPHA (='Aqueous Phase')

Function:

a. Performs aqueous phase calculations.

b. Evaluates H^+ in cloud and rain.

c. Performs gas/cloud partitioning of SO_2, HNO_3, NH_3, and HOOH.

d. Evaluates mass transfer rates between gas and rain of SO_2, HNO_3, NH_3, and HOOH.

e. Evaluates SO_2 oxidation rates in cloud and rain.

****

Subroutine DISSCON (='Dissociation constants')

Function:

a. To calculate dissociation and Henry's Law Constants for SO_2, HNO_3, NH_3, CO_2, O_3, HOOH.

b. Documentation of code to be described by Easter (1986).

****

Subroutine AQEQUIL (='Aqueous Equilibrium')

Function:

a. Calculates H^+ concentration.

b. Gas/aqueous partitioning based on equilibrium solubility, partitioning of aqueous phase species.

c. Documentation of code to be described by Easter (1986).

Key Algorithms:

a. Gases included are SO_2, CO_2, HNO_3, O_3, HOOH, NH_3 and formaldehyde.

****

Subroutine AQNONEQ3 (='Aqueous Non-Equilibrium, Version 3')

Function:

a. Rain-water aqueous chemistry routine.

b. Calculates H^+ concentration, gas/aqueous partitioning based on equilibrium solubility (for SO_2 and O_3).

c. Partitions aqueouse phase species.

d. Documentation of code to be described by Easter (1986).

Key Algorithms:

a. Gases included are: SO_2, CO_2, HNO_3, O_3, HOOH, NH_3 and formaldehyde.

****

Subroutine METSUM (='Meteorological Summary')

Function:

a. To print out summary of meteorological and scavenging environment in the RSM.

User Interaction:

a. None. In the present form of the RSM, this subroutine is called at the end of every simulation.

Key Algorithms:

a. When called, the following information is printed to file FOR006:[1]
   1. T, I_RADM, J_RADM
   2. J_GRID, AREA(J_GRID)
   3. K,
   4. X(3,K) (km)
   5. WINDS(1,J_GRID,K)
   6. R(1,J_GRID,K,KTEMP) - 273.15 (C)
   7. PTOT(1,J_GRID,K)/1000 (mb)
   8. CAIR(1,J_GRID,K)

[1]Units of printed values are as indicated in glossary unless noted otherwise.

9. R(1,J_GRID,K,KCLOUD)*CAIR(1,J_GRID,K)*18E6 (g/m^3)
10. R(1,J_GRID,K,KRAIN)*CAIR(1,J_GRID,K)*18E6 (g/m^3)
11. R(1,J_GRID,K,KSNOW)*CAIR(1,J_GRID,K)*18E6 (g/m^3)
12. VERTCL(1,J_GRID,K,2)
13. VERTCL(1,J_GRID,K,3)
14. RATE(J_GRID,K,KAUTO)
15. RATE(J_GRID,K,KMELT)
16. RATE(J_GRID,K,KEVAP)
17. RATE(J_GRID,K,KFREEZ)
18. RATE(J_GRID,K,KDEP)
19. RATE(J_GRID,K,KRIM)
20. RATE(J_GRID,K,KSUB)
21. RATE(J_GRID,K,KACCRET)
22. R(1, J_GRID,K,KVAPCL)

****

Subroutine CHEMSUM (='Chemistry Summary')

Function:

a. To print out summary of chemical environment in the RSM.

User Interaction:

a. None. In the present form of the RSM, this subroutine is called at the end of every simulation.

Key Algorithms:

a. When called, the following information is printed to file FOR006:[1]
   1. T, I_RADM, J_RADM
   2. R(1,J_GRID,K,L) for L = 1, LTOT2

****

Subroutine MASS_SUM (='Mass Summary')

Function:

a. To calculate the total mass being simulated in the scavenging module.

---

[1]Units of printed values are as indicated in glossary unless noted otherwise.

b. To print the results of this calculation by partitioning the sum according to major groups of species.

c. The results are intended to provide the user with a measure of how much mass has been "lost" as a result of the numerical integration.

User Interaction:

a. None. In the present form of the scavenging module, this subroutine is called once before the numerical integration starts, and immediately after the numerical integration is completed.

Key Algorithms:

a. The following values are printed to file FOR006:[1]

1. NAME, TOTAL (moles/cm^2) and OLDTOTAL (moles/cm^2) for every species simulated in the scavenging module.

2. (TOTAL-OLDTOTAL)/OLDTOTAL, (dimensionless) a measure of the fractional change in mass for every species in the scavenging module for which OLDTOTAL does not = 0.

In the following list, DELTAxxx refers to the total change in mass of the quantity being described (Delta = final - initial).

DELTA_xxx(J) refers to the mass removed by wet scavenging in cell J. [See entry for Subroutine DELTA_MASS)]

3. SO2 and DELTASO2, DELTA_SO2(J) (mass associated with $SO_2|gc$, $SO_2|s$ and $SO_2|r$)

4. PEROXIDES and DELTAPEROXIDE, DELTA_HOOH (mass associated with HOOH|gc, HOOH|r, HOOH|s)

5. SO4 and DELTASO4, DELTA_SO4(J) (mass associated with $SO_4|a1c$, $SO_4|a2$, $SO_4|r$ and $SO_4|s$)

6. CATN and DELTACATN (mass associated with CATN|a1c, CATN|a2, CATN|r and CATN|s)

[1]Units of printed values are as indicated in glossary unless noted otherwise.

7. FNITRATES and DELTAN, DELTA_NO3(J) (mass associated with NO_3|galc, NO_3|a2, NO_3|r and NO_3|s)

8. AMMONIA and DELTAA, DELTA_NH4(J) (mass associated with NH_4|galc, NH_4|a2, NH_4|r and NH_4|s)

9. SULFUR and DELTASULF, DELTA_SO2(J) + DELTA_SO4(J) (mass associated with SO_2 and SO_4 (defined in 3. and 5. above))

10. O3HOOHSO4 and DELTAO3, DELTA_HOOH(J) + DELTA_SO4(J) (mass associated with O_3|g, PEROXIDES and SO_4 (defined in 4. and 5. above).

****

Function THICK (='Thickness of layer')

Function:

a. To define the thickness of any layer given a height index and an array of elevation values.

b. Thickness defined in this way assures consistency throughout the scavenging module.

Key Algorithms:

a. The top layer has a thickness defined by one half the difference in height beteen top of the scavenging module grid, and the height of the top of the penultimate layer.

b. The bottom layer has a thickness defined by one half the difference in height between the top of the second lowest layer, and the height of the lowest layer.

c. Other layers have a thickness equal to one half the difference in elevation of two adjacent layers.

****

Subroutine DATADUMP (='Data Dump')

Function:

a. To write data from key arrays to file FOR001. These values will be used in the Type II Benchmark Tests described in Section 5.

****

Subroutine CORE (='core program to numerical integration')

Function:

a. To govern subroutines involved with the numerical integration component of the scavenging module.

b. Documentation to be provided by Hales (1988).

Key Algorithms:

a. Time splitting results in the following sequence of calculations:

1. Horizontal transport between scavenging module columns simulated for 1 delta-t intervals,

2. Vertical transport in each scavenging module column simulated for 1 delta-t intervals,

3. Local change (chemistry) in each scavenging module column simulated for 2 delta-t intervals,

4. Vertical transport in each scavenging module column simulated for 1 delta-t intervals,

5. Horizontal transport between each scavenging module column simulated for 1 delta-t interval.

****

Subroutine DELTA_MASS (='Delta mass with time')

Function:

a. To evaluate the mass removed by wet removal at every integration step.

b. To evaluate of Eq. 27 for major categories of species (see section 2.4.

Key Algorithms:

a. Evaluation of the pollutant mass wet that has been removed at a given time step is done by expressions of the form:

```
WET_xx = 2.*DT*CAIR(1,J,1) * VERTCL(1,J,1,2)*R(1,J,1,KXXXR)
```

where xx represents: SO_2, SO_4, NH_4 or HOOH

2.*DT is the time step local integration. (see Subroutine CORE). CAIR converts mixing ratio to moles/cm^3.

b. Evaluation of the total mass change in a column (moles/cm^2) between calls to MASS_SUM is given by expressions of the form:

```
DELTA_xxx(J) = DELTA_xxx(J) + WET_xxx(j)
c                           + (PHI(KxxxC) + PHI(KxxxR)
c                           +  PHI(KxxxS))*2.*DT
```

where xxx represents: SO_2, HOOH, SO_4, NO_3 or NH_4 and PHI represents ϑ in Eq. 25 (see Subroutine ENTRANSUM)

User Interaction:

a. if KDIAG > 0, the following quantities are printed to file FOR006:[1]
   1. J_GRID, I_RADM, J_RADM, T and 2.*DT
   2. CAIR(1,J,1), VERTCL(1,J,1,2), VERTCL(1,j,1,3)
   3. R(1,j,1,KxxxR), R(1,J,1,KxxxS) (xxx as defined above)
   4. WET_xxx(J) (xxx as defined above)
   5. DELTAΣxxx(j) (xxx as defined above)

****

Subroutine ENTRANSUM (='Entrainment summation')

Function:

a. To evaluate phi in Eq. 25.

Key Algorithms:

a. PHI(K) is reinitialized at the start of the subroutine.

b. Embedded within a DO loop over height are the terms.

```
DO 20 JFROM = 1, JTOT
DO 20 JTO   = 1, JTOT
IF (JFROM .NE. JTO)
+    SUMFLUX(K) = SUMFLUX(K) + F(K,JFROM,JTO) - F(K,JTO, JFROM))
20   CONTINUE
```

[1]Units of printed values are as indicated in glossary unless noted otherwise.

c. Since SUMFLUX is independent of species, the following DO loop over species (contained within a DO loop over height) will evaluate phi:

```
DO L = 1, LTOT
PHI(L) = PHI(L) + R(1,J,K,L) * SUMFLUX(K) * DZ/AREA(J)
END DO
```

User Interaction:

a. If KDIAG > 0, the following values are printed out:[1]
   1. K
   2. Z(K) (km)
   3. SUMFLUX(K)
   4. PHI(L), L = 1, LTOT

****

Subroutine YINTEG (='Y (horizontal Integration')

Function:

a. To simulate horizontal transport of material between cells in the scavenging module.

b. Theoretical development of this subroutine is contained in section 2.2 of this report.

Design Limitations:

a. See section 2.2, in particular, that section dealing with the definition of fluxes.

Key Algorithms:

a. Expressions to evaluate Eq. 10 are of the general form:

```
DO L = 1, LTOT                    (loop over computed species)
DO K = 1, KTOT                    (loop over height)
IF(AREA(J_GRID) .GT. .001)        (check if RSM cell J_GRID is used)
+    R(1,J_GRID,K,L) = R(1,J_GRID,K,L) -
                       (DT/AREA(J_GRID)*CAIR(1,J,K))*
+                          (R(1,J,K,L) * F(J,1,K)
+                       + R(1,J+1,K,L) * F(J+1,1,K)
+                       + R(1,J+2,K,L) * F(J+2,1,K)
+                       + R(1,J+3,K,L) * F(J+3,1,K)
```

[1]Units of printed values are as indicated in glossary unless noted otherwise.

```
     +                                  - R(1,J,K,L) * (F(1,J,K) + F(1,J+1,K) +
     +                                                  F(1,J+2,1,K) + F(1,J+3,K)))
                              *
                              *
     (similar calculations for other values of J_GRID)
                              *
                              *
     END DO
     END DO
```

User Interaction:

a. If KDIAG > 0, then the flux values are printed to file FOR006:
   1. F(JDET,JENT,K), JDET = detrainment grid index
                      JENT = entrainment grid index